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The doublet representation of non-Hilbert eigenstates of the Hamiltonian

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We find the minimal mathematical structure to represent quantum eigenstates with complex eigenvalues with no need of analytic continuation. These eigenvectors build doublets in non-Hilbert spaces. We construct exact solutions for the Friedrichs model that continuously join the ones of the free Hamiltonian. We extend the Wigner operator to these non-Hilbert spaces and enlarge the concept of normalized vectors via the definition of the doublets. Making use of these doublets, we describe systems whose states have initial conditions out of Hilbert space. © 1996 American Institute of Physics. [S0022-2488(96)00204-4]

I. INTRODUCTION

As it is generally known, unstable quantum states can be rigorously represented by (Gamow) vectors of rigged Hilbert spaces defined using Hardy class functions.^{1–4} Then a natural question arises: is this the most general rigorous mathematical model for unstable quantum states?

The aim of this paper is to find the minimal mathematical structure to represent quantum states in non-Hilbert spaces and to conjecture a provisional definition of probability for them. In this approach we describe the states in an eigenbasis of the free Hamiltonian $\{|1\rangle, |\omega\rangle\}$, where ω $(0 \le \omega \le \infty)$ is the frequency which represents the energy of the system and $|1\rangle$ is a discrete eigenstate of eigenvalue $\omega_0 > 0$.

We know that the eigenvalue problem for unbounded self-adjoint operators is not solvable in Hilbert space.⁵ The Gelfand–Maurin theorem^{6–8} deals with this problem and allows the appearance of eigenvalues that belong eventually to the complex plane. This is the case, for example, of the Hamiltonian of a discrete harmonic oscillator coupled to a bath described by the Fredrichs model which is usually solved by analytic continuation (and, in this case, there are unstable quantum states that belong to the above mentioned rigged Hilbert space^{9–14}) or by perturbation methods.¹⁵

In this work we construct exact solutions for the Friedrichs model that are continuous in the coupling constant. This is a desirable property of the solutions we are looking for. In other words, we would like to bypass the Poincaré cathastrophe¹⁶ generalized to the quantum domain. Then, all the solutions emerge in a natural way, with no need of analytic continuations¹⁷ or perturbative methods¹⁵ and they belong to a vector space that contains Hilbert space \mathscr{H} . This extended space is defined by the construction itself. Rigged Hilbert space will be a particular case of this construction and we believe that it encompasses other mathematical structures where unstable quantum states can be rigorously defined (nuclear spaces or convex algebras of operators¹⁸).

Furthermore, as the extended wave functions do not belong to Hilbert space any more, they lose their usual role in the probabilistic interpretation. Making use of the Friedrichs example, we

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introduce a doublet, namely the wave function plus a partner wave function, both belonging to convenient extended spaces, which seems to yield a criterion for extending the definition of probability.

The paper is organized as follows: in Sec. II we show that the requirement of continuity in the coupling parameter implies the appearance of complex eigenvalues. In Sec. III we define an operation (the star operation) which assigns a real number to the components of the doublet in generalized spaces. Section IV is devoted to well posing the Hamilton equations in the new space and in Sec. V we find the spectrum of the Hamiltonian. In Sec. VI we discuss the relation between the star operation and an extension of the time reversal Wigner operator. In Sec. VII we discuss the problem of defining probabilities and finding mean values in non-Hilbert spaces. In Sec. VIII we give a brief resume of the results. In Appendix A we show that our treatment allows us to recover the non-pure-exponential decay in Hilbert space. In Appendix B we study the statistics of a non-Hilbert eigenvector and its corresponding energy.

II. COMPLEX EIGENVALUES AND ANALYTICITY IN THE COUPLING PARAMETER

In this section we study the consequences of demanding a well-behaved $\lambda \rightarrow 0$ limit for the eigenvectors and eigenvalues of the Friedrichs Hamiltonian *H*. This Hamiltonian reads

$$H = H_0 + H_{\text{int}},\tag{1}$$

where

$$H_0 = \omega_0 |1\rangle \langle 1| + \int_0^\infty \omega |\omega\rangle \langle \omega| d\omega$$

is the free Hamiltonian,

$$H_{\rm int} = \lambda \int_0^\infty g(\omega) [|\omega\rangle \langle 1| + |1\rangle \langle \omega|] d\omega,$$

 ω_0 is the discrete eigenvalue, $\omega \in \Re^+$ is the continuous spectrum, and the eigenvectors of the free Hamiltonian satisfy

$$\langle 1|1\rangle = 1, \quad \langle 1|\omega\rangle = \langle \omega|1\rangle = 0, \quad \langle \omega|\omega'\rangle = \delta(\omega - \omega'),$$

 $\lambda \in \Re$ and the interaction $\lambda g(\omega)$ causes transitions between the discrete and continuous states. Let $|\psi\rangle$ be a vector belonging to the vector space Ξ spanned by the eigenvectors of H_0 , the space where H_0 and H are defined,

$$|\psi\rangle = \varphi_1|1\rangle + \int_0^\infty \varphi(\omega)|\omega\rangle, \quad |\psi\rangle \in \Xi,$$
(2)

where

$$\varphi_1 = \langle 1 | \psi \rangle$$
 and $\varphi(\omega) = \langle \omega | \psi \rangle$.

In Hilbert space \mathcal{H} , where quantum mechanics of stable states is formulated, the coefficients satisfy

$$\varphi_1 \varphi_1^* + \int_0^\infty \varphi(\omega) \varphi^*(\omega) d\omega < \infty$$
(3)

(* indicates complex conjugation). With this condition, \mathcal{H} and its conjugated space have the topology of the norm. Nevertheless, as H_0 and H are unbounded continuous operators, we can relax condition (3) to work in the less restrictive vector space $\Xi \supset \mathcal{H}$.

In terms of wave functions, we have the evolution equations

$$\langle 1|H|\psi\rangle = \omega_0\varphi_1 + \lambda \int g(\omega)\varphi(\omega)d\omega = i \frac{\partial}{\partial t}\varphi_1, \qquad (4)$$

$$\langle \omega | H | \psi \rangle = \omega \varphi(\omega) + \lambda g(\omega) \varphi_1 = i \frac{\partial}{\partial t} \varphi(\omega).$$
(5)

As (4) and (5) are true for any $|\psi\rangle$, we have

$$\langle 1|H = \omega_0 \langle 1| + \lambda \int_0^\infty g(\omega) \langle \omega| d\omega = \langle 1|i \frac{\partial}{\partial t}, \qquad (6)$$

$$\langle \omega | H = \omega \langle \omega | + \lambda g(\omega) \langle 1 | = \langle \omega | i \frac{\partial}{\partial t}.$$
 (7)

If we call $\langle \tilde{1} |$ and $\langle \tilde{\omega} |$ the left eigenstates of *H*, we have

$$\langle \tilde{1} | H = \tilde{\omega}_0 \langle \tilde{1} | = \langle \tilde{1} | i \frac{\partial}{\partial t}, \qquad (8)$$

$$\langle \widetilde{\omega} | H = \widetilde{\omega} \langle \widetilde{\omega} | = \langle \widetilde{\omega} | i \, \frac{\partial}{\partial t}, \tag{9}$$

H being a self-adjoint operator acting on \mathcal{H} and $\widetilde{\omega}_0, \ \widetilde{\omega} \in \mathfrak{R}$.

To obtain the vectors that diagonalize the Hamiltonian, let $\langle 1|, \langle \omega|$ and $\langle \widetilde{1}|, \langle \widetilde{\omega}|$ be linked by the ansatz

$$\langle \tilde{1} | = \xi \langle 1 | + \int_0^\infty \phi(\omega) \langle \omega | d\omega, \qquad (10)$$

$$\langle \widetilde{\omega} | = \xi_{\widetilde{\omega}} \langle 1 | + \int_0^\infty \phi_{\widetilde{\omega}}(\omega) \langle \omega | d\omega.$$
 (11)

Taking into account that we have not defined a topology in Ξ , all we can demand of the vectors with respect to the continuous parameter λ is that

$$\lim_{\lambda \to 0} \langle \tilde{1} | \psi \rangle = \langle 1 | \psi \rangle, \tag{12}$$

$$\lim_{\lambda \to 0} \langle \widetilde{\omega} | \psi \rangle = \langle \omega | \psi \rangle, \tag{13}$$

 $\forall |\psi\rangle \epsilon \Xi$ and

$$\lim_{\lambda \to 0} \widetilde{\omega}_0 = \omega_0. \tag{14}$$

For short we will write (12) and (13) as

$$\lim_{\lambda \to 0} \langle \tilde{1} \rangle = \langle 1 \rangle, \tag{15}$$

$$\lim_{\lambda \to 0} \langle \widetilde{\omega} | = \langle | \omega, \tag{16}$$

and refer to them as "the weak limits."

The ansatz (10) and (11) plus the dynamical evolution lead to the following equations for the coefficients ξ , $\phi(\omega)$:

$$(\widetilde{\omega}_0 - \omega_0) = \lambda \int_0^\infty \phi(\omega) g(\omega) d\omega, \qquad (17)$$

$$(\widetilde{\omega}_0 - \omega)\phi(\omega) = \xi \lambda g(\omega). \tag{18}$$

If $\widetilde{\omega}_0 \in \mathfrak{R}^+$, the solution to (17) and (18) is

$$\phi(\omega) = \delta(\widetilde{\omega}_0 - \omega) + \frac{\lambda g(\omega)}{(\widetilde{\omega}_0 - \omega \pm i\epsilon)}.$$
(19)

This solution should be rejected because when replacing (19) in (10) the δ -function causes the undesired behavior

$$\lambda = 0 \Longrightarrow \langle \widetilde{1} | = \xi \langle 1 | + \langle \omega_0 | \neq \langle 1 |.$$
⁽²⁰⁾

Therefore to guarantee that the δ -function disappears from $\phi(\omega)$, $\tilde{\omega}_0$ must not belong to \Re^+ . In this case we have

$$\phi(\omega) = \frac{\lambda g(\omega)}{(\tilde{\omega}_0 - \omega)}.$$
(21)

Replacing (21) in (17) we have the condition

$$\alpha(\widetilde{\omega}_0) \cdot \xi = 0 \quad \text{with} \quad \alpha_{\pm}(\omega) = \omega_0 - \omega - \lambda^2 \int_0^\infty \frac{g^2(\omega')d\omega'}{\omega \pm i\epsilon - \omega'}, \tag{22}$$

where

$$\alpha_{+}(\omega) - \alpha_{-}(\omega) = -2\pi i \lambda^{2} g^{2}(\omega).$$
⁽²³⁾

If α were different from zero, ξ had to be zero, and we would have again, in Eq. (10), the undesired behavior

$$\lambda = 0 \Longrightarrow \langle \widetilde{1} | \neq \langle 1 |.$$

So we need $\alpha(\widetilde{\omega}_0) = 0$.

In this section we have considered only real eigenvalues. Therefore, reminding the reader that the eigenvalue $\tilde{\omega}_0$ does not belong to \Re^+ , if $\tilde{\omega}_0$ is real, it must belong to \Re^- . However, as $\omega_0 > 0$, when λ approaches continuously 0, $\tilde{\omega}_0$ goes through the forbidden zone $\tilde{\omega}_0 > 0$. So we conclude that there is no acceptable $\tilde{\omega}_0$ real solution. Then the root $\tilde{\omega}_0$ of $\alpha(\omega)=0$ must be complex and it cannot be an eigenvalue of a self-adjoint Hamiltonian operator over \mathcal{H} .

III. THE STAR OPERATION

In order to diagonalize the Hamiltonian preserving continuity in λ , we reformulate the problem from the very beginning, namely, from the field equations (6)–(9). Let us define the space Ξ' of the linear functionals over Ξ

$$F(\varphi_1,\varphi(\omega))=n\epsilon \mathscr{C}$$

where $(\varphi_1, \varphi(\omega))$ are the components of vector $|\psi\rangle \epsilon \Xi$. In space Ξ , in spite of the fact that we have lost the notion of normalizability, a physical meaningful concept of probability can be defined all the same as we shall see. To do this, let us define a mapping \star on vectors of Ξ :

$$\star : \Xi \to \Xi'$$

$$\star : (\varphi_1, \varphi(\omega)) \to (\varphi_1, \varphi(\omega))^{\star} \equiv (\varphi_1^{\star}, \varphi^{\star}(\omega)),$$

$$F_{(\varphi_1, \varphi(\omega))}((\varphi_1, \varphi(\omega))) = \varphi_1 \varphi_1^{\star} + \int_0^\infty \varphi(\omega) \varphi^{\star}(\omega) = \langle \psi^{\star} | \psi \rangle$$

satisfying

- (a) $F_{(\varphi_1,\varphi(\omega))}((\varphi_1,\varphi(\omega)))$ is a (finite) number constant in time and
- (b) $[(\varphi_1,\varphi(\omega))^{\star}]^{\star} = (\varphi_1,\varphi(\omega))$. Then vector

$$|\psi\rangle = \varphi_1 |1\rangle + \varphi(\omega) |\omega\rangle$$

and its partner

$$\langle \psi^{\star} | = \varphi_1^{\star} \langle 1 | + \varphi^{\star}(\omega) \langle \omega | = F_{(\varphi_1, \varphi(\omega))}(\cdot),$$

whose coefficients obey conditions (a) and (b), are said to belong to the spaces Φ and Φ^* . These spaces satisfy $\mathcal{H} \subset \Phi \subset \Xi$ and $\mathcal{H}' \subset \Phi^* \subset \Xi'$. (We will show in Appendix B that there is at least one vector in Φ which does not belong to \mathcal{H} .) Properties (a) and (b) make bra $\langle \psi^* |$ a convenient partner of ket $|\psi\rangle$ in order to define probabilities.

Of course, if $|\psi\rangle \in \mathcal{H}$ we have that

$$\langle \psi^{\star} | = \langle \psi |, \quad \varphi_1^{\star} = \varphi_1^{\star}, \text{ and } \varphi^{\star}(\omega) = \varphi^{\star}(\omega),$$

and the usual state of affairs is reproduced.

As we shall see in Sec. IV, the time evolution of φ_1^* and $\varphi^*(\omega)$ is completely determined by the action of the Hamiltonian over φ_1 and $\varphi(\omega)$ and conditions (a) and (b).

IV. FIELD EQUATIONS IN THE EXTENDED SPACE $\Phi{\oplus}\Phi^{\star}$

We demand the action of the "partner" of the Hamiltonian, namely H^* , which determines the temporal evolution of $F_{(\varphi_1,\varphi(\omega))}$ to satisfy

$$H^{\star}F_{(\varphi_1,\varphi(\omega))}(\varphi_1,\varphi(\omega)) = F_{(\varphi_1,\varphi(\omega))}(H(\varphi_1,\varphi(\omega))).$$
(24)

In order to find it explicitly, we use the fact that the temporal evolution of $(\varphi_1, \varphi(\omega))$ is given by (4) and (5) and the independence of time requested by condition (a) of Sec. III. Then, in components, Eq. (24) reads

$$\omega_{0}\varphi_{1}\varphi_{1}^{\star} + \lambda \int_{0}^{\infty} g(\omega)\varphi(\omega)\varphi_{1}^{\star}(\omega)d\omega + \int_{0}^{\infty} \omega\varphi(\omega)\varphi^{\star}(\omega)d\omega + \lambda \int_{0}^{\infty} g(\omega)\varphi_{1}\varphi^{\star}(\omega)d\omega$$
$$= -i\varphi_{1}\partial_{t}\varphi_{1}^{\star} - i\int_{0}^{\infty} \varphi(\omega)\partial_{t}\varphi^{\star}(\omega)d\omega, \qquad (25)$$

which splits into

$$\omega_0|1\rangle + \lambda \int_0^\infty g(\omega)|\omega\rangle d\omega = (-i) \frac{\overline{\partial}}{\partial t}|1\rangle, \qquad (26)$$

$$\omega|\omega\rangle + \lambda g(\omega)|1\rangle = (-i) \frac{\overline{\partial}}{\partial t}|\omega\rangle, \qquad (27)$$

which are nothing but the ket version of (6) and (7) ($\overline{\partial}$ indicates left derivative).

Now we want to obtain the diagonal form of the complete set of equations in the $\Phi \oplus \Phi^*$ extended space of doublets $\{|\psi\rangle, \langle\psi^*|\}$. The set of equations for the bras has the same form as (8) and (9) but, in order to indicate that the Hamiltonian eigenvalues may be complex, we call them $\widetilde{z_0}, \widetilde{z}$ instead of $\widetilde{\omega_0}, \widetilde{\omega}$:

$$\langle \tilde{1}|H = \tilde{z}_0 \langle \tilde{1}| = \langle \tilde{1}|i \frac{\partial}{\partial t}, \qquad (28)$$

$$\langle \widetilde{z} | H = \widetilde{z} \langle \widetilde{z} | = \langle \widetilde{z} | i \frac{\partial}{\partial t}.$$
(29)

The ket set of the diagonal equations is obtained from Eq. (24) using (28) and (29). They are

$$H^{\star}|\tilde{1}\rangle = \tilde{z}_{0}|\tilde{1}\rangle = (-i) \frac{\overline{\partial}}{\partial t}|\tilde{1}\rangle, \qquad (30)$$

$$H^{\star}|\tilde{z}\rangle = \tilde{z}|\tilde{z}\rangle = (-i)\frac{\overline{\partial}}{\partial t}|\tilde{z}\rangle.$$
(31)

Kets $|\tilde{1}\rangle$, $|\tilde{z}\rangle$ are the right eigenvectors of H^{\star} .

We want to emphasize that, in general, $\langle \widetilde{1} | \neq (|\widetilde{1}\rangle)^*$ and $\langle \widetilde{z} | \neq (|\widetilde{z}\rangle)^*$, i.e., $\langle \widetilde{1} |$ and $\langle \widetilde{z} |$ are not necessarily the partners of $|\widetilde{1}\rangle$, $|\widetilde{z}\rangle$. Indeed, the star operation is not always well defined among the right and left eigenvectors of H.

V. THE SPECTRUM OF THE HAMILTONIAN

The Friedrichs model has been long treated in the literature. Recently, in Ref. 15, it was found a basis that diagonalized the Hamiltonian preserving continuity in the coupling parameter λ using a perturbative method. On the other hand, in Ref. 17 an exact solution was obtained regardless of the continuity in λ .

Here we find a diagonal basis for the same problem that it is not only an exact solution but also preserves the desired continuity in λ . In order to diagonalize the Hamiltonian we will use an ansatz to relate the diagonal and nondiagonal basis, namely,

$$\langle \tilde{1} | = \xi \langle 1 | + \int_0^\infty \phi(\omega) \langle \omega | d\omega, \qquad (32)$$

$$|\tilde{1}\rangle = \xi^{\star}|1\rangle + \int_{0}^{\infty} \phi^{\star}(\omega)|\omega\rangle d\omega, \qquad (33)$$

$$\langle \widetilde{z} | = \xi_{\widetilde{z}} \langle 1 | + \int_{0}^{\infty} \phi_{\widetilde{z}}(\omega) \langle \omega | d\omega, \qquad (34)$$

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$$|\tilde{z}\rangle = \xi_{\tilde{z}}^{\star}|1\rangle + \int_{0}^{\infty} \phi_{\tilde{z}}^{\star}(\omega)|\omega\rangle d\omega.$$
(35)

Applying the Hamiltonian to the ansatz (32)–(35) we obtain

$$\phi(\omega) = \xi \, \frac{\lambda g(\omega)}{\widetilde{z_0} - \omega}, \quad \phi^*(\omega) = \xi^* \, \frac{\lambda g(\omega)}{\widetilde{z_0} - \omega},$$
$$\xi \left(\omega_0 - \widetilde{z_0} - \lambda^2 \int_0^\infty \frac{g^2(\omega)}{\widetilde{z_0} - \omega} \, d\omega \right) = 0 \Rightarrow \alpha(\widetilde{z_0}) = 0.$$

Requiring the good behavior with respect to λ , the coefficient $\phi_{\tilde{z}}(\omega)$ results:

$$\phi_{\tilde{z}}(\omega) = \delta(\tilde{z} - \omega) + \xi_{\tilde{z}} \frac{\lambda g(\omega)}{\tilde{z} - \omega}.$$
(36)

Here $\delta(\tilde{z}-\omega)$ is the δ -function generalized to complex numbers. This extension of Dirac's δ -function as mentioned by Gelfand and Shilov¹⁹ goes beyond the tempered distributions and was used by Nakanishi²⁰ in the discussion of the Friedrichs model. In order to preserve the good limit, $\delta(\tilde{z}-\omega)$ must be different from zero for every \tilde{z} , i.e., $\{\tilde{z}\}$ must coincide with \mathfrak{R}^+ . So we call $\tilde{\omega}$ this real variable:

$$\phi_{\widetilde{\omega}}(\omega) = \delta(\widetilde{\omega} - \omega) + \xi_{\widetilde{\omega}} \frac{\lambda g(\omega)}{\widetilde{\omega} - \omega}, \qquad (37)$$

$$\xi_{\widetilde{\omega}}(\widetilde{\omega} - \omega_0) = \lambda g(\widetilde{\omega}) + \xi_{\widetilde{\omega}} \lambda^2 \int_0^\infty \frac{g^2(\omega)}{\widetilde{\omega} - \omega} \, d\omega, \tag{38}$$

i.e.,

$$\xi_{\widetilde{\omega}} = \frac{\lambda g(\widetilde{\omega})}{\alpha(\widetilde{\omega})} \quad \text{and} \quad \phi_{\widetilde{\omega}}(\omega) = \delta(\widetilde{\omega} - \omega) + \frac{\lambda^2 g(\omega) g(\widetilde{\omega})}{(\widetilde{\omega} - \omega) \alpha(\widetilde{\omega})}.$$

The singularities in $\alpha(\tilde{\omega})$ and $(\tilde{\omega}-\omega)^{-1}$ must be avoided making the shift $\pm i\epsilon$. We do not write it explicitly so as not to embarrass the notation. The equivalent star equations to (37) and (38) yield

$$\xi_{\widetilde{\omega}}^{\star} = \frac{\lambda g(\widetilde{\omega})}{\alpha(\widetilde{\omega})}$$

and

$$\phi_{\widetilde{\omega}}^{\star}(\omega) = \delta(\widetilde{\omega} - \omega) + \frac{\lambda^2 g(\omega) g(\widetilde{\omega})}{(\widetilde{\omega} - \omega) \alpha(\widetilde{\omega})}.$$

Putting it all together, the change of basis that diagonalizes the Hamiltonian results in

$$\langle \tilde{1} | = \xi \langle 1 | + \xi \int_0^\infty \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega} \langle \omega | d\omega, \qquad (39)$$

$$|\tilde{1}\rangle = \xi^{\star}|1\rangle + \xi^{\star} \int_{0}^{\infty} \frac{\lambda g(\omega)}{\tilde{z}_{0} - \omega} |\omega\rangle d\omega, \qquad (40)$$

$$\left\langle \widetilde{\omega} \right| = \frac{\lambda g(\widetilde{\omega})}{\alpha(\widetilde{\omega})} \left\langle 1 \right| + \int_0^\infty \left[\delta(\widetilde{\omega} - \omega) + \frac{\lambda^2 g(\omega) g(\widetilde{\omega})}{(\widetilde{\omega} - \omega) \alpha(\widetilde{\omega})} \right] \left\langle \omega \right| d\omega, \tag{41}$$

$$\left|\widetilde{\omega}\right\rangle = \frac{\lambda g\left(\widetilde{\omega}\right)}{\alpha(\widetilde{\omega})} \left|1\right\rangle + \int_{0}^{\infty} \left[\delta(\widetilde{\omega} - \omega) + \frac{\lambda^{2} g\left(\omega\right) g\left(\widetilde{\omega}\right)}{\left(\widetilde{\omega} - \omega\right) \alpha(\widetilde{\omega})}\right] \left|\omega\right\rangle d\omega, \tag{42}$$

where

$$\left[\xi\xi^{\star}\right]^{-1} = \frac{\partial\alpha(z)}{\partial z}\bigg|_{z=\tilde{z}_{0}} \equiv \alpha'$$

When the initial conditions belong to \mathcal{H} , solutions (39)–(42) are such that temporal evolution keeps the state into \mathcal{H} . As we have already said, $\langle \tilde{\omega} |$ of Eq. (41) must be understood as $\langle \tilde{\omega} \pm |$ and the same for $|\tilde{\omega}\rangle$ of Eq. (42). Taking this into account, a straightforward computation proves that they are nothing but the retarded and advanced Lippman–Schwinger solutions, which are exact solutions of the Friedrichs model.²¹

We will also need the inverse of the ansatz. To obtain it, we posed the inverse problem and, after some calculation, we obtained

$$\langle 1| = \eta \langle \widetilde{1}| + \int_0^\infty \frac{\lambda g(\widetilde{\omega})}{\alpha(\widetilde{\omega})} \langle \widetilde{\omega}| d\widetilde{\omega}, \qquad (43)$$

$$|1\rangle = \eta^{\star} |\tilde{1}\rangle + \int_{0}^{\infty} \frac{\lambda g(\tilde{\omega})}{\alpha(\tilde{\omega})} |\tilde{\omega}\rangle d\tilde{\omega}, \qquad (44)$$

$$\langle \omega | = \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega} \eta \langle \tilde{1} | + \int_0^\infty \left[\delta(\omega - \tilde{\omega}) + \frac{\lambda^2 g(\omega) g(\tilde{\omega})}{(\tilde{\omega} - \omega) \alpha(\tilde{\omega})} \right] \langle \tilde{\omega} | d\tilde{\omega}, \tag{45}$$

$$|\omega\rangle = \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega} \eta^* |\tilde{1}\rangle + \int_0^\infty \left[\delta(\omega - \tilde{\omega}) + \frac{\lambda^2 g(\omega) g(\tilde{\omega})}{(\tilde{\omega} - \omega) \alpha(\tilde{\omega})} \right] |\tilde{\omega}\rangle d\tilde{\omega}.$$
(46)

The composition of the transformations (39)-(42) and (43)-(46) gives the identity transformation, so one is the inverse of the other. Having found a regular transformation which has a regular inverse, we conclude that we have found a new basis for the space $\Phi \oplus \Phi^*$ and also the spectrum of the Hamiltonian.

VI. THE STAR OPERATION AND TIME REVERSAL

In order to avoid the difficulties of the bra-ket notation when dealing with antilinear operators,²² we will use the wave function formalism to generalize the time reversal operator and to compare it with the star operation.

We know that in \mathcal{H} the action of the time reversal operator T, in the wave function formalism, comes from the conjugation of the Schrödinger equation, i.e., we have

$$T: \mathcal{H} \to \mathcal{H},$$
$$\varphi \to \varphi^* \quad \text{and} \ t \to -t.$$

In Φ , Schrödinger equations (28)–(31) (with $\tilde{z} = \tilde{\omega}$) in the wave function formalism read

$$H\widetilde{\varphi}_1 = \widetilde{z}_0 \widetilde{\varphi}_1 = i \,\frac{\partial}{\partial t} \,\widetilde{\varphi}_1, \qquad (47)$$

$$H\widetilde{\varphi}(\widetilde{\omega}) = \widetilde{\omega}\widetilde{\varphi}(\widetilde{\omega}) = i \frac{\partial}{\partial t} \widetilde{\varphi}(\widetilde{\omega}), \tag{48}$$

$$H^{\star} \widetilde{\varphi}_{1}^{\star} = \widetilde{z}_{0} \widetilde{\varphi}_{1}^{\star} = -i \, \frac{\partial}{\partial t} \, \widetilde{\varphi}_{1}^{\star}, \tag{49}$$

$$H^{\star}\widetilde{\varphi}^{\star}(\widetilde{\omega}) = \widetilde{\omega}\widetilde{\varphi}^{\star}(\widetilde{\omega}) = -i\frac{\partial}{\partial t}\widetilde{\varphi}^{\star}(\widetilde{\omega}).$$
(50)

As we can immediately see, in the extended space the appearance of complex eigenvalues forces the time reversal to be related to the star operation which is not a simple complex conjugation. In the extended space we can define an extension of T,

$$\widetilde{T}:\Phi \rightarrow \Phi^{\star}, \quad \widetilde{T}^{-1}:\Phi^{\star} \rightarrow \Phi,$$

whose action can be represented by

$$\varphi \rightarrow \varphi^{\star}$$
 when $t \rightarrow -t$.

On the other hand, as $\tilde{z_0} = \tilde{\omega_0} - i \gamma/2$ with $\gamma \in \Re^+$ (conventionally), solution to Eq. (47),

$$\widetilde{\varphi}_1(t) = \widetilde{\varphi}_1(0) \exp(-i\widetilde{z}_0 t) = \widetilde{\varphi}_1(0) \exp(-i\widetilde{\omega}_0 t) \exp(\gamma t/2),$$

is not defined when $t \rightarrow \infty$. Analogously, solution to Eq. (49),

$$\widetilde{\varphi}_{1}^{\star}(t) = \widetilde{\varphi}_{1}^{\star}(0) \exp(i\widetilde{z}_{0}t) = \widetilde{\varphi}_{1}^{\star}(0) \exp(i\widetilde{\omega}_{0}t) \exp(-\gamma t/2),$$

is not defined when $t \to -\infty$. So, temporal evolution described by Eqs. (47)–(50) is not defined in the whole interval $[-\infty, \infty]$ but in $[-\infty, \infty)$ for solutions which evolve with H and in $(-\infty, \infty]$ for those which evolve with H^* . This fact could be related to the splitting of the system evolution group into two semigroups¹⁵ for the case of non-pure states and will be studied elsewhere.

VII. DISCUSSION ABOUT PROBABILITY AND MEAN VALUE OF OBSERVABLES IN EXTENDED SPACES

In this section we will sketch a discussion about a possible probabilistic interpretation for our extended formalism. Consider that the system is initially free and that the self-interaction begins at t=0 and finishes at an arbitrary time t, when the system becomes free again. During the interaction, eigenvalues of the operator H may be complex and states represented by $|\psi\rangle$ and $\langle\psi\star|$ may also belong to the extended space. In order to define probability in this space we consider again the scalar quantity

$$\langle \psi^{\star} | \psi \rangle = \varphi_1 \varphi_1^{\star} + \int_0^{\infty} \varphi(\omega) \varphi^{\star}(\omega) d\omega = \langle \widetilde{\psi}^{\star} | \widetilde{\psi} \rangle = \widetilde{\varphi}_1 \widetilde{\varphi}_1^{\star} + \int_0^{\infty} \widetilde{\varphi}(\widetilde{\omega}) \widetilde{\varphi}^{\star}(\widetilde{\omega}) d\widetilde{\omega}$$
(51)

that we have introduced in Sec. III to construct the space Φ^* and we normalize it to 1. Here $\langle \psi^* | \psi \rangle$ is a scalar conserved under the change of basis and constant in time and reduces to the standard norm when $|\psi\rangle$ belongs to \mathcal{H} . However, we cannot be assured that each term of Eq. (51) is a real

number. Nevertheless, if it is so, we are able to interpret each term of the sum (51) as a probability itself, i.e., $\varphi_1(t)\varphi_1^{\star}(t)$ represents the probability of finding the system in the discrete eigenstate of the free Hamiltonian and

$$\int_{\omega}^{\omega+\Delta\omega}\varphi(\omega,t)\varphi^{\star}(\omega,t)d\omega$$

represents the probability of finding the system in the continuous spectrum with frequencies into $[\omega, \omega + \Delta \omega]$ after the interaction. In this case, we have a natural extension of the definition of probability from \mathcal{H} to the extended space $\Phi \oplus \Phi^*$.

Notice that, even in cases in which the \star operation is well defined in the extended space and is conserved in time and under changes of basis, these facts are not enough to guarantee that the first term and any partial integral in the sum (51) belong to the interval [0, 1]. As it was pointed out,²³ we can interpretate this fact as being related with initial conditions not possible to be realized or representing a situation for which probability cannot be verified directly or a combination of both. These situations would be impossible, not in the sense that the chance for their occurrence is zero, but in the sense that the conditions of preparation or verification of those states are unattainable. The problem of an adequate interpretation of negative probabilities has been long studied. See, for example, Refs. 23 and 24.

With our definition of probability the mean value of a constant of motion A is defined as

$$\overline{A} = \sum_{i} a_{i} P(\varphi_{i}) + \int a \mathscr{P}(\varphi(a)) da = \sum_{i} a_{i} \varphi_{i} \varphi_{i}^{\star} + \int a \varphi(a) \varphi^{\star}(a) da,$$

where a_i and a belong to the discrete and continuous spectra of A, respectively. \overline{A} is in general a complex number and reduces to a real one when A is a self-adjoint operator on \mathcal{H} . Notice that when the eigenvalues a_i are positive real numbers, the mean value \overline{A} is a positive real number if probability also is. This allows us to have states with positive defined unperturbed energy out of \mathcal{H} . Namely, even in the extended space, when the initial conditions are so that their corresponding probabilities belong to [0, 1], we can guarantee the positivity of the mean value of the unperturbed energy \overline{H}_0 :

$$\overline{H_0} = \omega_0 |1\rangle \langle 1| + \int_0^\infty \omega |\omega\rangle \langle \omega| d\omega.$$

So we can relate reality and positivity of probability with positivity of this energy. It is in this sense that we have said that negative probabilities correspond to impossible initial conditions.

Regardless our interpretation is merely a conjecture we will use to see how it works in two cases: in Appendix A the conjecture applied to a Hilbert space vector lets us reproduce the non-pure exponential decay. In Appendix B we use the conjecture to compute probabilities and mean values of energy for a system whose initial conditions are out of \mathcal{H} .

VIII. CONCLUSIONS

We have found an exact solution of the Friedrichs model which for the continuous spectrum coincides with the Lippman–Schwinger solutions. To find the right and left eigenvectors of the Hamiltonian with interaction, we have neither made use of analytic continuations nor perturbative methods. As we have preserved continuity in the coupling parameter λ , our approach is also applicable to systems that must be treated in a perturbative way. We also found the minimal mathematical structure to represent quantum states. To generalize the notion of probability from \mathcal{H} , we defined the star operation in Sec. III and constructed the doublets of wave functions. The star operation is also related to the time reversal operation in the extended space. The main tool

that we have is the scalar magnitude defined by Eq. (51). This scalar magnitude, built up with a doublet of wave functions, plays in the extended space an analogous role to the norm in \mathcal{H} and reduces to it when the star operation reduces to the conjugation. Then we have a probabilistic interpretation of this extension of the norm. Further restrictions conducing to the choice of a particular topology will be imposed when they appear necessary because of physical reasons. In a forthcoming work we will try to apply our formalism to more realistic models like those of Refs. 25-29.

Finally we show in Appendix A that our approach gives the correct non-purely exponential decay amplitude and, in Appendix B, our formalism is applied to describe quantum states out of \mathcal{H} .

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APPENDIX A: THE NON-PURE EXPONENTIAL DECAY

Here we apply our formalism to study the decay of a state whose initial condition belongs to \mathcal{H} and that represents, at t=0, a particle with energy ω_0 :

$$\langle 1| = \begin{pmatrix} \varphi_1 = 1 \\ \varphi(\omega) = 0 \end{pmatrix}.$$

Then, as $\langle 1 |$ belongs to \mathcal{H} , we have

$$(\langle 1|)^{\star} \equiv |1^{\star}\rangle = |1\rangle = \begin{pmatrix} \varphi_1^{\star} = 1\\ \varphi^{\star}(\omega) = 0 \end{pmatrix}.$$

Temporal evolution in the diagonal basis is

$$\widetilde{\varphi}_{1}(t) = \frac{1}{\sqrt{\alpha'}} e^{-i\widetilde{z}_{0}t}, \quad \widetilde{\varphi}_{1}^{\star}(t) = \frac{1}{\sqrt{\alpha'}} e^{i\widetilde{z}_{0}t},$$
$$\widetilde{\varphi}(\widetilde{\omega}, t) = \frac{\lambda g(\widetilde{\omega})}{\alpha(\widetilde{\omega})} e^{-i\widetilde{\omega}t}, \quad \widetilde{\varphi}^{\star}(\widetilde{\omega}, t) = \frac{\lambda g(\widetilde{\omega})}{\alpha(\widetilde{\omega})} e^{i\widetilde{\omega}t}.$$

So, in the nondiagonal basis, the wave functions are

$$\langle 1|1(t)\rangle = \varphi_1(t) = \frac{e^{-i\widetilde{z}_0 t}}{\alpha'} + \int_0^\infty \frac{\lambda^2 g^2(\widetilde{\omega})}{\alpha^2(\widetilde{\omega})} e^{-i\widetilde{\omega} t} d\widetilde{\omega},$$
$$\langle 1^*(t)|1\rangle = \varphi_1^*(t) = \frac{e^{i\widetilde{z}_0 t}}{\alpha'} + \int_0^\infty \frac{\lambda^2 g^2(\widetilde{\omega})}{\alpha^2(\widetilde{\omega})} e^{i\widetilde{\omega} t} d\widetilde{\omega}.$$

Changing the contours of integration appropriately (see Appendix A of Ref. 17) and Eq. (23), $\varphi_1(t)$ results in

$$\varphi_1(t) = -\frac{i}{2\pi} \int_{\Gamma} \frac{e^{-izt}}{\alpha(z)} dz.$$

With our definition, the probability of having the system in the discrete state is $\varphi_1 \varphi_1^*$. By direct computation it can be seen that

$$\varphi_1^{\star}(t) \!=\! \varphi_1^{\star}(t)$$

as corresponds to a vector belonging to \mathcal{H} . So

$$\varphi_1 \varphi_1^\star = \varphi_1 \varphi_1^\star = |\varphi_1|^2$$

predicts the correct non-pure exponential decay amplitude with the $\rm Zeno^{30,31}$ and Khalfin effects. 32,33

APPENDIX B: PROBABILITY AND UNPERTURBED ENERGY OF A NON-HILBERT EIGENSTATE

We consider now a system whose initial state is the discrete eigenstate of *H* with eigenvalue $\widetilde{z_0}$:

$$\langle \tilde{1}| = \begin{pmatrix} 1\\ 0 \end{pmatrix}. \tag{B1}$$

Given (B1), its partner satisfying Eq. (51) is

$$(\langle \widetilde{1} |)^{\star} \equiv | \widetilde{1}^{\star} \rangle = | \widetilde{1} \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Temporal evolution gives

$$\left[\begin{pmatrix} e^{-i\widetilde{z}_0t}\\0 \end{pmatrix}, \begin{pmatrix} e^{i\widetilde{z}_0t}\\0 \end{pmatrix}\right].$$

In terms of the eigenfunctions of the free Hamiltonian, the doublet reads

$$\varphi_1(t) = \frac{1}{\sqrt{\alpha'}} e^{-i\tilde{z}_0 t}, \quad \varphi_1^{\star}(t) = \frac{1}{\sqrt{\alpha'}} e^{i\tilde{z}_0 t}, \tag{B2}$$

$$\varphi(\omega) = \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega} \frac{1}{\sqrt{\alpha'}} e^{-i\tilde{z}_0 t}, \quad \varphi^{\star}(\omega) = \frac{\lambda g(\omega)}{\tilde{z}_0 - \omega} \frac{1}{\sqrt{\alpha'}} e^{i\tilde{z}_0 t}.$$
 (B3)

As (B2) and (B3) are solutions of the Schrödinger equations that do not belong to Hilbert space, they need to be given a physical interpretation.

First we check the conservation of probability:

$$\widetilde{\varphi}_{1}\widetilde{\varphi}_{1}^{\star} + \int_{0}^{\infty} \widetilde{\varphi}(\widetilde{\omega}) \widetilde{\varphi}^{\star}(\widetilde{\omega}) d\widetilde{\omega} = 1$$

and

$$\varphi_1\varphi_1^{\star} + \int_0^{\infty} \varphi(\omega)\varphi^{\star}(\omega)d\omega = \frac{1}{\alpha'} + \int_0^{\infty} \frac{1}{\alpha'} \frac{\lambda^2 g^2(\omega)}{(\tilde{z}_0 - \omega)^2} d\omega = \frac{1}{\alpha'} + \frac{\alpha' - 1}{\alpha'} = 1$$

because

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$$\alpha = z - \omega_0 - \lambda^2 \int_0^\infty \frac{g^2(\omega)}{(z - \omega)} d\omega \Rightarrow \frac{\partial \alpha(z)}{\partial z} \bigg|_{z = \tilde{z}_0} = \alpha' = 1 + \lambda^2 \int_0^\infty \frac{g^2(\omega)}{(\tilde{z}_0 - \omega)^2} d\omega.$$

With this procedure we have a way to identify a pure state corresponding to a complex eigenvalue in terms of the eigenfunctions of the free Hamiltonian: it is a state with probability $1/\alpha'$ of being in the discrete level with energy ω_0 and probability $(\alpha'-1)/\alpha'$ of being in any level ω of the continuum, respectively. These probabilities are constant in time as it corresponds to an eigenstate of \mathcal{H} .

We now compute the mean value of the energy when the interaction finishes:

$$\overline{H}_{0(\widetilde{\varphi}_{1},\widetilde{\varphi}_{1}^{\star})} = \omega_{0}\varphi_{1}\varphi_{1}^{\star} + \int_{0}^{\infty} \omega\varphi(\omega)\varphi^{\star}(\omega)d\omega.$$
(B4)

Using (B2) and (B3) we have

$$\overline{H}_{0(\widetilde{\varphi}_{1},\widetilde{\varphi}_{1}^{\star})} = \frac{1}{\alpha'(\widetilde{z}_{0})} \left(\omega_{0} + \int_{0}^{\infty} \omega \, \frac{\lambda^{2} g^{2}(\omega)}{(\widetilde{z}_{0} - \omega)^{2}} \, d\omega \right). \tag{B5}$$

Some comments are in order:

- (1) \overline{H}_0 is a real number if probability is.
- (2) If the interaction $g(\omega)$ is such that $(\tilde{\varphi}_1, \tilde{\varphi}_1^*)$ is a possible initial condition, the unperturbed energy of the state is a positive number.
- (3) When $\lambda \rightarrow 0$, we have the correct limit $\lim_{\lambda \rightarrow 0} \overline{H}_0 = \omega_0$.
- (4) The mean value of the evolution operator during the interaction that corresponds to $(\tilde{\varphi}_1, \tilde{\varphi}_1^*)$ state is the complex number $\overline{H}_{(\tilde{\varphi}_1, \tilde{\varphi}_1^*)} = \tilde{z}_0$. This is not surprising because it is only the evolution operator and the energy is not defined during the interaction.

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