Fulfillment of unitarity for the non-Hermitian decaying probability density involving the full set of resonance states to the Schrödinger equation

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By using an exact analytical non-Hermitian formalism involving the full set of resonance (quasinormal) states and complex energy eigenvalues for quantum tunneling decay, we show that unitarity holds at any instant of time for the nonstationary decaying probability density in the whole space, thus providing a fundamental description of the quantum mechanical decay process.

I. INTRODUCTION

In conventional quantum mechanics the time evolution operator is unitary because the Hamiltonian is Hermitian. As a consequence, the eigenvalues are real and the norm of the evolving state remains constant in time, a fact that reflects the physical requirement of conservation of probability. The above consideration seems to be in contradiction with approaches that describe the norm of the evolving state remains constant in time, thus providing a fundamental description of the quantum mechanical decay process.

Let us briefly review some relevant developments on the description of quantum tunneling decay since the early days of quantum mechanics. In 1928, Gamow imposed outgoing (radiative) boundary conditions on the solutions to the time-dependent Schrödinger equation by considering a problem where he replaced the complicated many-body nuclear potential by a single-particle potential from which the α-particle decays by tunneling. From time-reversal considerations he obtained that the solutions for positive energies are discrete and have complex energy eigenvalues \( E_n = \mathcal{E}_n - i\Gamma_n/2 \) [1, 2]. In addition to a probability density that decays exponentially with time at each point of space, it turns out that beyond the interaction region, the amplitude of these states increases exponentially with distance and therefore the usual rules of normalization and completeness do not apply for these states. Separation of variables leads to complex energy solutions to the time-independent Schrödinger equation

that have been used to describe sharp resonances in scattering processes [6–8]. Since the imaginary part of the energy determines both the width of the resonance and the decay constant in the time evolution of decay, these states are commonly named resonance states, though other names as Gamow states, quasinormal states, and Siegert states for time-independent processes, have also been used [9].

Around the sixties of last century, Khalfin pointed out, following a theorem by Paley and Wiener [10], that the exponential decay law cannot hold at all times and showed that there must be a transition to decay as an inverse power of time [11]. Some years later it was also shown that at short-times compared with the lifetime, the decay deviates also from exponential decay, typically exhibiting a \( t^2 \) behavior [12], see however, Ref. [13]. The short-time behavior of decay has attracted a lot of attention regarding the quantum Zeno effect [14–17]. So one sees therefore, that the description of quantum tunneling decay has become more complex than in Gamow’s time. Also, with the advent of artificial quantum structures, one may manipulate the potential parameters of the decaying systems to investigate the time of transition from one regime to another [18, 19].

The second half of the last century also witnessed some relevant theoretical developments regarding resonance states. These were influenced by rigorous developments regarding the analytical properties of the outgoing Green’s function [20]. Various approaches led to similar normalization rules [21–24] and distinct resonance expansions [9, 24–26] and also to mathematically oriented studies on rigged Hilbert spaces [27–32] or the extension of the the Lax-Phillips theory to quantum mechanics [33–35], to describe decaying systems.

The present work addresses the issue of unitarity in quantum tunneling decay for potentials that vanish beyond a distance using a resonance-state expansion valid in the interval \((0, a)\), with \(a\) the potential radius, which involves the full set of resonance states and complex poles of the outgoing Green’s function of the problem [9, 36]. We show analytically, for each value of time, that the decaying probability density is quadratically integrable and therefore unitarity is preserved. This is in contrast with common approaches involving resonance expansions that hold in the interval \([0, \infty)\) involving only proper complex poles, i.e. \( \mathcal{E}_n > \Gamma_n/2 \), as in Gamow’s approach. There,
resonance states grow exponentially with distance and hence lead to a description that is manifestly non-unitary \cite{37}.

Our approach refers to the full Hamiltonian to the problem and hence it differs from approaches where the Hamiltonian $H$ is written as $H = H_0 + H_1 + H_{\text{int}}$ where $H_0$ a closed system that couples by $H_{\text{int}}$, to an environment $H_1$ to become an open system. In these treatments the decay process is usually treated to some degree of perturbation theory, as in the work by Weisskopf and Wigner on the exponential decay of an excited atom interacting with a quantized radiation field \cite{38}, and in studies on the deviation of exponential decay in these systems \cite{39}.

The paper is organized as follows. Section II reviews some relevant properties of resonance states, which involve the complex poles of the propagator and the resonance (quasinormal) states to the problem and discuss the time evolution of the decaying solution. In Sec. III we analyze the asymptotic behavior of the decaying solution as a function of distance for fixed values of time. In Sec. IV, we exemplify our findings using an exactly solvable model, and finally, Sec. V presents some concluding remarks.

II. FORMALISM

Here we recall the relevant aspects of the derivation of the decaying wave solution for a single particle confined initially within the internal region of a spherically symmetric real potential with the condition, imposed on physical grounds, that it vanishes beyond a distance, i.e., $V(r) = 0$ for $r > a$. We choose natural units $\hbar = 2m = 1$ and for simplicity of the discussion and without loss of generality we consider a $s$-wave Hamiltonian to the system $H = -\frac{d^2}{dr^2} + V(r)$. The solution to the time-dependent Schrödinger equation may be written in terms of the retarded Green’s function $g(r, r'; t)$ of the problem as \cite{9},

$$
\Psi(r, t) = \int_0^a g(r, r'; t)\Psi(r', 0) \, dr',
$$

where $\Psi(r, 0)$ stands for an arbitrary initial state which is confined within the internal interaction region. Since the decay refers to tunneling into the continuum, for the sake of simplicity it is assumed that the potential does not possess bound nor antibound states. The retarded time-dependent Green’s function $g(r, r'; t)$ is the relevant quantity to study the time evolution of the initial state for $t > 0$ and may be evaluated by a Laplace transformation into the complex wave number plane $k$,

$$
g(r, r'; t) = \frac{i}{2\pi} \int_{C_0} G^+(r, r'; k)e^{-ik't} 2dk,
$$

where the Bromwich contour $C_0$ corresponds to a hyperbolic contour along the first quadrant of the $k$ plane that may be deformed, in the absence of bound states as assumed here without loss of generality, to a contour that goes from $-\infty$ to $\infty$ along the real $k$ axis, namely,

$$
g(r, r'; t) = \frac{i}{2\pi} \int_{-\infty}^{\infty} G^+(r, r'; k)e^{-ikt} 2dk.
$$

A consequence of the condition that the potential vanishes after a distance is that $G^+(r, r'; k)$ may be extended analytically to the whole complex $k$ plane where it has an infinite number of complex poles distributed on the third and fourth quadrants symmetrically with respect to the Im-$k$ axis \cite{20}.

Resonance states are the solutions to the radial Schrödinger equation,

$$
[E_n - H]u_n(r) = 0,
$$

obeying outgoing (radiative) boundary conditions,

$$
u_n(r) = A_n e^{i\kappa_n r}, \quad r \geq a,
$$

where $\kappa_n = \alpha_n - i\beta_n$ and $E_n$ stands for the complex energy eigenvalues,

$$
E_n = \kappa_n^2 = \mathcal{E}_n - i\Gamma_n/2,
$$

where $\mathcal{E}_n = \alpha_n^2 - \beta_n^2$ represents the resonance energy of the decaying particle and $\Gamma_n = 4\alpha_n\beta_n$ the corresponding resonance width. As is well known, the longest lifetime sets up the time scale of the decay process. Resonance states may be obtained also from the residues $\rho_n(r, r')$ at the complex poles $\{\kappa_n\}$ of the outgoing Green’s function to the problem $G^+(r, r'; k)$ \cite{9, 24, 40}, namely,

$$
\rho_n = \frac{u_n(r)u_n(r')}{2\kappa_n},
$$

provided the following normalization condition is satisfied,

$$
\int_0^a u_n^2(r)dr + \frac{i\kappa_n^2(a)}{2\kappa_n} = 1.
$$

It may be shown that (8) is equivalent to the normalization convention proposed by Zel’ dovich \cite{41}.

Let us now, following Refs. \cite{26, 42}, consider the integral,

$$
J = \frac{1}{2\pi i} \int_C \frac{G^+(r, r'; k')}{k'^2 - k} \, dk',
$$

where $C$ represents a large closed contour in the $k$ plane around the origin of radius $R$, that includes also the closed contours within $C$, $c_k$, around an arbitrary real value $k' = k$, and the sum of contours around the poles $\kappa_n$ and $\kappa_{-n}$, located on the fourth and third quadrants of the $k$ plane, namely, $C = C_R + c_k + \sum \kappa_n$. Since the contour $C$ excludes all singularities, it follows from Cauchy’s theorem that $J = 0$ and hence, applying the theorem of
residues to evaluate the distinct contours, using (7), one
is left with the expression,
\[ G^+(r, r'; k) = \sum_{n=-N}^{N} \frac{u_n(r)u_n(r')}{2\kappa_n(k-k_n)} \]
and the sum rules,
\[ \sum_{n=-\infty}^{\infty} \frac{u_n(r)u_n(r')}{\kappa_n} = 0, \quad (r, r') \leq a, \quad (13) \]
and
\[ \sum_{n=-\infty}^{\infty} u_n(r)u_n(r')\kappa_n = 0, \quad (r, r') \leq a, \quad (14) \]
which play a significant role to derive the short and long-
time behaviors in the time evolution of decay [9, 36].

Using the identity \[ 1/[2\kappa_n(k-k_n)] \equiv (1/2k)[1/(k-k_n) + 1/\kappa_n] \}
one may write (11), in view of (13) as,
\[ G^+(r, r'; k) = \frac{1}{2k} \sum_{n=-\infty}^{\infty} \frac{u_n(r)u_n(r')}{k-k_n} \]
\[ \quad \quad \quad \quad \quad (r, r') \leq a, \quad (15) \]
Then, substitution of (15) into (3) and then into (1) allow
us to write the time-dependent decaying wave function
\[ \Psi(r, t) \quad \text{for} \quad r \leq a. \]

Using the expression of \( G^+(r, r'; k) \)
in terms of the regular and irregular solutions to the
Schrödinger equation [20], one may easily obtain the
identity,
\[ G^+(r, r'; k) = G^+(r', a; k)e^{ik(r-a)}, \quad r' < a, \quad r \geq a. \quad (16) \]
Then considering (15) one may expand \( G^+(r', a; k) \)
in terms of the full set of resonance states and substituting
the resulting expression into (3) and then into (1), leads
to the resonance expansion of the decaying wave function
\( r' < a \) and \( r \geq a \). Hence, we may write the decaying
wave solution as [9, 36],
\[ \Psi(r, t) = \begin{cases} 
\Psi_{in}(r, t), \quad r \leq a, \\
\Psi_{ex}(r, t), \quad r \geq a,
\end{cases} \quad (17) \]
where \( \Psi_{in}(r, t) \) and \( \Psi_{ex}(r, t) \) are given by,
\[ \Psi_{in}(r, t) = \sum_{n=-\infty}^{\infty} C_n u_n(r)M(y_n^o), \quad r \leq a \quad (18) \]
and
\[ \Psi_{ex}(r, t) = \sum_{n=\infty}^{\infty} C_n u_n(a)M(y_n), \quad r \geq a, \quad (19) \]
with the coefficients \( C_n \) in the above two expressions
given by,
\[ C_n = \int_0^a \Psi(r, 0)u_n(r)dr. \quad (20) \]
The functions \( M(y_n) \) in (19) are defined as [9, 36],
\[ M(y_n) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{ik(r-a)}e^{-ik^2t}}{k-\kappa_n} \]
\[ \quad = \frac{1}{2}e^{i(r-a)^2/4t}w(iy_n), \quad (21) \]
\[ \quad = \frac{1}{2}e^{i(r-a)^2/4t}e^{y_n^2}\text{erfc}(y_n) \]
with
\[ y_n = e^{-i\pi/4}(1/4t)^{1/2}(r-a-2\kappa_nt). \quad (22) \]
The functions \( w(z) = \exp(-z^2)\text{erfc}(-iz) \) in (21) stand for the
Faddeyeva-Terent’ev or complex error function [44]
for which there exist computational tools to calculate it
[45]. The argument \( y_n^o \) of the functions \( M(y_n^o) \) in (18) is
that of \( y_n \) with \( r = a \), namely,
\[ y_n^o = e^{-i\pi/4}\kappa_n^{1/2}. \quad (23) \]
It is worth mentioning that putting \( \kappa_n = k' \), with \( k' \) a
real value in (22), yields the function \( M(y_n') \) introduced
by Moshinsky in his study of the phenomenon of diffraction in time for the transient propagation of a free particle [46, 47]. This phenomenon was extended to potentials of finite range in one dimension by García-Calderón and Rubio using the full set of resonance states [40]. There, the internal and propagating solutions for the tunneling transient process are given in terms of the functions $M(y_n^0)$ and $M(y_n)$ defined above. The function $M(y_n)$ has also been used to describe the propagation of a decaying particle without considering explicitly resonance states [48].

### A. Analysis of the time evolution of the decaying solution

#### 1. Internal resonance solution

Let us first refer to the time evolution of the decaying solution along the internal region of the potential $r \leq a$ $\Psi_{in}(r,t)$ given by (18). By using the symmetry relations mentioned above, among the poles and resonance states located on the third quadrant with those on the fourth quadrant on the $k$ plane, namely, $\kappa_{-n} = \kappa_n^*$ and $u_{-n}(r) = u_n^*(r)$ allows us to write $\Psi_{in}(r,t)$ as,

$$\Psi_{in}(r,t) = \sum_{n=1}^{\infty} [C_n u_n(r) M(y_n^0) + \bar{C}_n u_n^*(r) M(y_n^0)].$$

One then may utilize a property of the functions $M(y_n^0)$ that establishes that,

$$M(y_n^0) = e^{-i\kappa_n^2 t} - M(-y_n^0),$$

provided that $\pi/2 < \arg(y_n^0) < 3\pi/2$ [9, 46]. This is in fact the case for resonance poles with $\alpha_n > \beta_n$, the so called proper resonance poles. The arguments of both $M(-y_n^0)$ and $M(y_n^0)$, satisfy $-\pi/2 < \arg(y_n^0) < \pi/2$, and as a consequence they do not exhibit an exponential behavior [9, 46]. As a result, one may write $\Psi_{in}(r,t)$ for $r \leq a$ as,

$$\Psi_{in}(r,t) = \sum_{n=1}^{\infty} C_n u_n(r) e^{-i\kappa_n^2 t} - e^{-\kappa_n^2 t/2} + I(r,t),$$

where $I(r,t)$ accounts for the nonexponential contribution [9],

$$I(r,t) = -\sum_{n=1}^{\infty} [C_n u_n(r) M(-y_n^0) - \bar{C}_n u_n^*(r) M(y_n^0)].$$

It is well known that the nonexponential term (27) is relevant at ultra short or very long times compared with the lifetime to the system. In the later case, for a real initial state $\Psi(r,0)$ and a given distance $r$ as a function of time it goes as [9, 36],

$$I(r,t) \approx i\eta \operatorname{Im} \left\{ \sum_{n=1}^{\infty} \frac{C_n u_n(r)}{\kappa_n^3} \right\} \frac{1}{t^{3/2}}; \quad r \leq a,$$

where $\eta = 1/(4\pi)^{1/2}$, exhibiting the well known long-time behavior as the inverse power of time $1/t^{3/2}$.

The decaying solution $\Psi_{in}(r,t)$, given by (26), is the relevant ingredient to calculate the survival probability $S(t) = |A(t)|^2$, where the survival amplitude $A(t)$ is a quantity that provides the probability amplitude that at time $t$ the decaying particle is still in the initial state,

$$A(t) = \int_0^a \Psi^*(r,0) \Psi(r,t) \, dr,$$

and the nonescape probability, which yields the probability that at time $t$ the decaying particle remains within the interaction region, namely,

$$P(t) = \int_0^a |\Psi(r,t)|^2 \, dr.$$

These two quantities have been discussed using the formalism of resonance states discussed here in a number of works [9, 36, 49–51]. One sees that the above quantities do not address the issue of the propagation of the decaying particle outside the interaction region. This is considered in the next Section.

#### 2. External resonance solution

For $r \geq a$, the solution $\Psi_{ex}(r,t)$, given by (19), describes the propagation of the decaying particle along the external region. This has been discussed in Refs. [9, 36, 52].

To discuss the propagation along the external region it is convenient to write (19), in a similar fashion as for the internal solution, to show explicitly the contributions corresponding to the third quadrant of the $k$ plane,

$$\Psi_{ex}(r,t) = \sum_{n=1}^{\infty} [C_n u_n(a) M(y_n) + \bar{C}_n u_n^*(a) M(y_n^0)].$$

The exponential and nonexponential behavior of $\Psi_{ex}(r,t)$ may be obtained in a similar fashion as in the case of $\Psi_{in}(r,t)$ given above, except that in the present case it depends on the overall sign of the argument $y_n$ given by (22) due to the presence of the term $(r-a)$. To clarify this, is convenient to write explicitly the real and imaginary parts of $y_n$ for a fixed time $t = t_0$, namely,

$$y_n = \frac{1}{2(2t_0)^{1/2}} \left[ (r-a) - 2(\alpha_n - \beta_n)t_0 \right]$$

$$- i \left[ (r-a) + 2(\alpha_n + \beta_n)t_0 \right]$$

that is, it depends on whether $(r-a)$ is larger or smaller than $2(\alpha_n - \beta_n)t_0$. Noticing that the imaginary part in (32) does not change sign, the case $(r-a) < 2(\alpha_n - \beta_n)t_0$ has an argument that satisfies $\pi/2 < \arg(y_n) < 3\pi/2$ and hence, in a similar fashion as for the internal case, it
exhibits an explicit exponential behavior, namely,

\[
\Psi_{ex}(r,t) = \sum_{n=1}^{\infty} C_n u_n(a)e^{i\kappa_n(r-a)}e^{-i(r-a)^2/4t}e^{-i\epsilon_n^2t}e^{-r-a/2} + J(r,t),
\]

(33)

where the nonexponential term reads,

\[
J(r,t) = -\sum_{n=1}^{\infty} \left[ C_n u_n(a)M(-y_n) - \bar{C}_n \bar{u}_n(a)M(y_n) \right].
\]

(34)

On the other hand, in the case \((r-a) > 2(\alpha_n - \beta_n)t_0\), a decomposition as that given in (33) no longer applies, since the argument \(y_n\) satisfies \(-\pi/2 < \arg(y_n) < \pi/2\), and hence the solution (31) behaves entirely in a nonexponential fashion.

As a consequence of the above considerations, one sees that the propagating solution \(\Psi_{ex}(r,t)\) grows exponentially in an oscillatory form until it reaches the value \((r-a) = 2(\alpha_n - \beta_n)t_0\), and subsequently it behaves in a nonexponential fashion. In the next Section we show analytically, for a given fixed time \(t_0\), that for large values of \(r\) the solution given by (31) goes as \(1/r\).

It is worth pointing out, in addition to the above discussion, that by assuming that the initial state \(\Psi(r,0)\) is normalized to unity, it follows from the closure relation (12) that,

\[
\text{Re} \sum_{n=1}^{\infty} \{ C_n \bar{C}_n \} = 1,
\]

(35)

where \(\bar{C}_n\) follows by taking the conjugate of \(\Psi(r,0)\) in (20). Equation (35) indicates that \(\text{Re} \{ C_n \bar{C}_n \}\) cannot be interpreted as a probability, since in general it is not a positive definite quantity. However, it may be seen as the ‘strength’ or ‘weight’ of the initial state in the corresponding resonant state.

III. ANALYSIS OF UNITARITY FOR THE DECAYING WAVE SOLUTION

Let us analyze the asymptotic behavior of the propagating decaying solution \(\Psi_{ex}(r,t)\) given in (19) for values \(r \geq a\), that is for asymptotically large values of \(r\). One sees immediately that the corresponding \(r\)-dependence is contained in the propagating function \(M(y_n)\), whose argument \(y_n\) is given by (22). It follows by inspection of this expression that for a given value of the time \(t, r \gg a\) implies

\[
|r| \gg |2\kappa_n t|,
\]

(36)

and hence \(y_n\) behaves as,

\[
y_n \approx \frac{1}{2} e^{-i\pi/4} \frac{1}{t^{1/2}} r.
\]

(37)

One then may obtain, in view of the right-hand side expression in (21), the asymptotic expansion of \(M(y_n)\) for \(|y_n| \gg 1\) [44],

\[
M(y_n) \approx \frac{1}{2} e^{i\pi/2} e^{i(\pi/2 + \pi/2)t} \left[ \frac{1}{\pi^{1/2}y_n} - \frac{1}{\pi^{1/2}y_n^3} + \ldots \right],
\]

(38)

to write the leading term of the decaying wave function \(\Psi(r,t)\) for \(r \gg a\) as,

\[
\Psi(r,t) \approx \frac{1}{\pi^{1/2}} e^{i\pi/4} e^{i\pi/2t} t^{1/2} \sum_{-\infty}^{\infty} C_n u_n(a) \frac{1}{r}.
\]

(39)

Since for \(t = 0\), in view of (21) and Eq. (7.1.8) of Ref. [44], \(M(y_n^0) = 1/2\), one may write,

\[
\sum_{-\infty}^{\infty} C_n u_n(a) = 2\Psi(r,0),
\]

(40)

and hence, asymptotically for \(|r| \gg a|\), the probability density may be written as,

\[
|\Psi_{ex}(r,t)|^2 \approx |\Psi(a,0)|^2 \frac{2t}{r^2},
\]

(41)

which shows that \(\Psi_{ex}(r,t)\) is quadratically integrable. Notice that in (41), the given value of \(t\) must satisfy (36).

The above considerations allow us, in view of (17), to define

\[
I_{in}(t) = \int_{0}^{a} |\Psi_{in}(r,t)|^2 dr,
\]

(42)
and
\[ I_{ex}(t) = \int_{0}^{\infty} |\Psi_{ex}(r,t)|^2 dr, \] (43)
so one may write the probability density integrated in the whole space, as
\[ \int_{0}^{\infty} |\Psi(r,t)|^2 dr = I_{in}(t) + I_{ex}(t). \] (44)
At the initial time \( t = 0 \), one has
\[ \int_{0}^{\infty} |\Psi(r,0)|^2 dr = I_{in}(0) = 1. \] (45)
As time evolves the initial probability density decays to the outside. However, since the potential is real, flux conservation is satisfied and hence probability is conserved. This means that if the initial state is normalized to unity, then at each instant of time \( t \) the following expression is satisfied,
\[ I(t) = \int_{0}^{\infty} |\Psi(r,t)|^2 dr = I_{in}(t) + I_{ex}(t) = 1. \] (46)
Equation (46) tell us that the non-Hermitian decaying probability density \( |\Psi(r,t)|^2 \), that follows from (17), satisfies the unitarity condition.

1. Comparison with Gamow’s and other resonance solutions

It may be of interest to make a comparison of the above results with Gamow’s approach along the external interaction region, where the propagating solution may be written as [1],
\[ \Psi_G(r,t) = [e^{i\alpha_n r}e^{-iE_n t}]e^{\beta r}e^{-\Gamma_n t/2}, \quad r \geq a, \] (47)
which shows analytically, as is well known, that for a given time it diverges with distance and hence it does not satisfy unitarity, namely,
\[ \int_{a}^{\infty} |\Psi_G(r,t)|^2 dr \rightarrow \infty. \] (48)
Notice that the solution (47) has a unity coefficient, which means that all other possible resonance solutions are excluded. A comparison of (47) with (31) exhibits the crucial role played by the nonexponential contributions to obtain the wavefront of the propagating resonance expansion of the decaying wave function discussed above.

Another solution of the decaying wave function has been given by García-Calderón and Peierls [24]. As discussed there, one may deform the Bromwich contour \( C_0 \) in Eq. (2) by a straight line 45° off the real \( k \) axis and a sum over the residues of the outgoing Green’s function at the complex poles located on the fourth quadrant of the \( k \) plane. Using the resulting expression into (3) yield for the decaying wave function,
\[ \Psi_{GCP}(r,t) = \sum_{n=1}^{\infty} C_n u_n(r)e^{-iE_n t}e^{-\Gamma_n t/2} + \int_{0}^{\infty} C(E)u(E,r)e^{-iEt} dE, \] (49)
where \( C(E) \) stands for the overlap of the initial state \( \Psi(r,0) \) with the complex energy continuum state \( u(E,r) \). The relevant point here is that for \( r > a \), each resonance term in (49) diverges with distance, and hence, as in Gamow’s case, the integrated probability density is manifestly non-unitary. Subsequent approaches close the contour \( C_0 \) in (2) in distinct forms to obtain finite or infinite number of resonance terms and different background integral contributions [37]. This includes the Rigged-Hilbert approach [31] and related approaches based on the extension of the Lax-Phillips formalism to describe quantum resonances [35]. A common model employed by these authors is the Friedrichs model [53] which has been primarily used to address the exponential decay of the survival probability.

It is relevant to emphasize that all the above resonance-state expansions involve, for \( t > 0 \), proper complex poles, i.e., those located on the fourth quadrant of the \( k \) plane, and hold in the interval \((0, \infty)\), whereas in the approach presented here the resonance expansion includes the full set of complex poles of the problem, i.e., involving the complex poles located on both the third and fourth quadrants of the complex \( k \) plane, and hold in the interval \((0, a)\). The above considerations summarize an essential difference of our approach with previous approaches.

2. Comparison with continuum wave expansions

It is worth mentioning that recently it has been shown that the time evolution of single-particle tunneling decay, for a fixed value of the distance as a function of time, involving the non-Hermitian full set of resonance states and that considering the Hermitian continuum wave functions yield identical results [36, 52]. An essential difference between these approaches is that the former provides analytical expressions for the different decaying regimes whereas the later consists of a ‘black-box’ numerical calculation. For example, the former provides exact analytical expressions for the exponential and long-time nonexponential regimes, as that given by (26) and (28), whereas the later involves the continuum wave functions \( \psi^+(k, r) \), which are the solutions to the Schrödinger equation to the problem,
\[ [E - H]\psi^+(k, r) = 0, \] (50)
where \( E = k^2 \), is a real energy and \( H \) is the Hamiltonian defined previously, namely \( H = -\frac{d^2}{dr^2} + V(r) \), that
appears in Eq. (4). As is well known, the Hamiltonian in this case is Hermitian. The continuum wave solutions \( \psi^+(k,r) \) are normalized to a Dirac delta and the set of functions \( \{\Psi^+(k,r)\} \) constitutes a complete orthonormal set.

For \( r \geq a \), the solution \( \psi^+(k,r) \) may be written as,

\[
\psi^+(k,r) = \sqrt{\frac{2}{\pi}} \frac{i}{2} \left[ e^{-ikr} - S(k)e^{ikr} \right], \quad r \geq a
\]

where \( S(k) \) is the S-matrix to the problem. It is also well known that for decay the time-dependent solution (1) may be written as an expansion involving the continuum wave functions, namely,

\[
\Psi(r,t) = \int_0^\infty C(k)\psi^+(k,r)e^{-ik^2t}dk,
\]

where the expansion coefficient \( C(k) \) is given by

\[
C(k) = \int_0^a \psi^{+\ast}(k,r')\Psi(r',0)dr',
\]

with \( \Psi(r',0) \) the initial state to the problem. Clearly, Eq. (52) does not provide any clue for the behavior of
IV. MODEL

As an example, let us consider the s-wave $\delta$-shell potential, which has shown to provide an excellent qualitative description of tunneling decay [36, 52, 54],

$$V(r) = \lambda \delta(r - a),$$  \hspace{1cm} (54)

where $\lambda$ stands for the intensity of the potential and $a$ for the radius. In our example we use $\lambda = 100$ and $a = 1$. The resonance solutions to the problem with complex energy eigenvalues $\kappa_n^2 = E_n - i\Gamma_n/2$ read,

$$u_n(r) = \begin{cases} A_n \sin(\kappa_n r) & r \leq a \\ B_n e^{i\kappa_n r}, & r \geq a, \end{cases}$$  \hspace{1cm} (55)

where we recall that $\kappa_n = \alpha_n - i\beta_n$. From the continuity of the above solutions and the discontinuity of its derivatives with respect to $r$ (due to the $\delta$-function interaction) at the boundary value $r = a$, it is obtained that the set of $\kappa_n$’s satisfy the equation,

$$2i\kappa_n + \lambda(e^{2i\kappa_n a} - 1) = 0.$$  \hspace{1cm} (56)

For $\lambda > 1$ one may write the approximate analytical solutions to Eq. (56) as [9]

$$\kappa_n \approx \frac{n\pi}{a} \left( 1 - \frac{1}{\lambda a} \right) - i \frac{1}{a} \left( \frac{n\pi}{\lambda a} \right)^2.$$  \hspace{1cm} (57)

One may solve numerically (56) by using iterative procedures as the Newton-Rapshon method, which allow us to calculate the complex poles $\kappa_n$ with the desired degree of approximation using the approximate solution given by (57) to generate the initial values. For a given value of the intensity $\lambda$ and a radius $a$ of the $\delta$-potential, one may then evaluate the corresponding set of complex poles $\{\kappa_n\}$ and the set of normalized resonance states $\{u_n(r)\}$.

We model the initially confined state by a given infinite box state,

$$\Psi(r, 0) = \sqrt{\frac{2}{a}} \sin \left( \frac{q\pi}{a} r \right), \quad q = 1, 2, 3...$$  \hspace{1cm} (58)

from which it is easy to obtain the expansion coefficients $\{C_n\}$ to the problem.

A relevant feature of the resonance formalism is that it provides exact analytic time-dependent solutions both in the internal region of the potential and along the external region. This allows us to see the time evolution of the decay of the initial state in the internal region and simultaneously the propagation along the external region.

Figure 1 provides a plot of $|\Psi_G(r, t)|^2$, given by (47), and $|\Psi_{ex}(r, t)|^2$, given by (19), as a function of the distance $r/a$ at the fixed time $t_0 = 0.5\tau$, with $\tau$ the lifetime of the system, to exhibit the exponential catastrophe of Gamow’s solution and the propagating wavefront of the resonance expansion solution. A similar figure has been presented in Ref. (48). It is worth pointing out that the resonance-state expansion for the propagating transmitted time-dependent solution of a double barrier resonant tunneling structure [40], looks similar to $|\Psi_{ex}(r, t)|^2$ in Fig. 1.

Figure 2 exhibits snapshots of the decay and propagation of the normalized initial state given by Eq. (58) for $q = 1$ (ground state of a quantum box). The left panel contains plots of the probability density $|\Psi_{in}(r, t)|^2$ vs $r$ in the confining internal region calculated from (18), whereas the right panel exhibits the corresponding plots of the propagating probability density $|\Psi_{ex}(r, t)|^2$ vs $r$, using (19), at each of the selected times $t$. The numerical values of $t$ are indicated in the upper right corner of each graph. This graphical representation allows the visualization of the time evolution of the probability density $|\Psi(r, t)|^2$ for quantum decay. We can see that as the probability density decreases inside the confining potential it grows and propagates along the external region with a wavefront which is situated at approximately the classical position $r_n = v_n t$ with $v_n = 2\alpha_n$. In the present case $n = 1$, which follows from the fact that the dominant term in the decay process corresponds to the coefficient $C_1^2 \approx 0.9$. We recall that the lifetime is given by $1/\Gamma_1$. The relevant point of Fig. 2 is that at each time $t$, Eq. (46) is essentially satisfied. By integrating numerically both (42) and (43), we calculate the values of $I_{in}(t)$ and $I_{ex}(t)$ indicated in each graph of fig. 2, and we obtain for each value of $t$, at least $I(t) = I_{in}(t) + I_{ex}(t) = 0.999$. In order to ensure a good approximation to the exact result, in our numerical integration we choose a long enough distance (up to $r/a = 4000$) along the tail on the right of the main wavefronts of Fig. 1. Although these tails look very smooth, they actually have a fine structure not visible in Fig. 1, as we show below making an appropriate zoom.
Figure 3 shows a zoom of the second graph of Fig. 2. It exhibits a succession of peaks whose wavefronts correspond to the contribution to decay of resonance levels corresponding to the high resonance energy levels. The distinct red dots, represent the position of the propagating resonance terms at the positions \( r_n \approx 2\alpha_n t \), with \( n = 2, 3, 4, \ldots \). There is, in fact, an infinite number of forerunners, in agreement with the nonrelativistic character of the formalism. It is worth mentioning the complexity exhibited by these propagating structures all of which contribute to the integral term \( I_{\text{ex}}(t) \) to ensure that the unitarity condition (46) is fulfilled.

Figure 4, in a similar fashion as in Fig. 2 for the initial state \( q = 1 \), exhibits snapshots of the decay and propagation of the normalized initial state given by Eq. (58) for \( q = 2 \) (second state of a quantum box). As can be seen on the left graphs of this figure, a transition from the decaying state \( q = 2 \) (characterized by two maxima) to the decaying state \( q = 1 \) (with a single maximum) occurs in the internal region. Initially, the decaying state is governed by the second resonance state of the system, whose main wavefront on the outside propagates at approximately the classical position \( r_2 = 2\alpha_2 t \) (clearly visible in each snapshot of Fig. 4). After the transition, the decaying state is the first resonance state of the system, and the corresponding wavefront is traveling behind the main wavefront. In view of the relatively small amplitude of the latter (since in this case \( C_1^2 \ll C_2^2 \approx 0.9 \)), we need to make a zoom on the graphs around the classical position \( r_1 = 2\alpha_1 t \) to see it. The inset on the last graph on the right of Fig. 4 exhibits such a traveling structure. In each snapshot shown in Fig. 4, the values of the integrals \( I_{\text{in}}(t) \) and \( I_{\text{ex}}(t) \) are also shown, and we can verify that Eq. (46) is satisfactorily fulfilled.

V. CONCLUDING REMARKS

We have shown that the non-Hermitian solution to the time-dependent Schrödinger equation given by Eqs. (17), (18) and (19), involving the full set of resonance eigenfunctions and complex wave number poles for the problem for the time evolution of tunneling decay, satisfies unitarity at each instant of time and hence conserves probability. The present result and recent work regarding the Heisenberg uncertainty relations involving resonance states [41] might be of particular interest for a line of inquiry that explores the possibility of extending the
standard formalism of quantum mechanics to incorporate in a fundamental fashion a non-Hermitian treatment of the Hamiltonian to the system for the description of open quantum systems.

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