Properties of the Expansion of the Decaying Wave Solution in Terms of Resonant States

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Abstract. We consider the formulation of quantum decay in terms of resonant states and complex poles of the outgoing Green's function of the problem to discuss some properties of the decaying wave solution that exhibit its non-Hermitian character and hence illustrate its departure from the standard formalism of quantum mechanics.

1. Introduction

In 1928, Gamow derived the analytical expression for the exponential decay law \( \exp(-\Gamma t/\hbar) \), with \( \Gamma \) the decay rate, by imposing purely outgoing boundary conditions to the solutions to the Schrödinger equation that describes the decaying system [1–3]. This was modeled by a potential having a barrier where the particle was initially confined prior to decay by tunneling into the open. The outgoing boundary conditions imply the vanishing of the coefficients of the incoming waves that appear in the solution to the Schrödinger equation outside the interaction region and lead, due to time-reversal considerations, to discrete complex energy eigenvalues. Purely outgoing boundary conditions imply a non-Hermitian formulation of decay. The vanishing of the incoming wave coefficients mentioned above corresponds to complex poles of the \( S \)-matrix to the problem. This led to formulations of nuclear reactions involving resonance expansions of the cross section [4, 5]. It is worth noticing, however, that this provides a link between the energy and the time domains, corresponding respectively, to scattering and decay, and to a definition of resonances as an intrinsic property of open quantum systems.

Around the fifties and sixties of last century it was shown that the exponential decay law cannot hold both at long times [6] and at very short times [7, 8] compared with the lifetime of the decaying system. The short-time behavior has been the subject of much discussion, particularly in connection with the quantum Zeno effect [9, 10]. Although the experimental search of departures from the exponential decay law remained elusive for decades [11], some years ago, however, it was verified in the short-time regime using ultracold atoms [12] and more recently, in the long-time regime, using organic molecules in solution [13]. The quantum Zeno effect has also been observed in ultracold decaying systems [14]. These experimental results seem to contradict theoretical claims made in the seventies of last century, that argued that due to the influence of the measurement apparatus on the decay process, the exponential decay law should hold at all times [15].

The theoretical description of tunneling decay is therefore more involved than in older times.
In general, it seems to consist of three regimes: Exponential and nonexponential at short and long times. The approach initiated by Gamow required of substantial modification to deal with the nonexponential contributions. At the end of the 1960s and along the 1970s there were some relevant developments on the properties of resonance states in the wave number domain that involved consideration of the analytical properties of the outgoing Green’s function to the problem [16]. The outgoing Green’s function provided an adequate framework to study the issues of normalization and eigenfunction expansions involving resonant states. The above considerations form the basis for the time-dependent treatment that I shall refer to below to describe the time evolution of decay. I will not refer here to other approaches, as the rigged-Hilbert approach recently reviewed in Ref. [17].

It might be worthwhile to point out that in recent work it is shown rigorously, using the analytical properties of the outgoing Green’s function for single particle potentials that vanish exactly beyond a distance, that the non-Hermitian formulation using resonance states and the Hermitian formulation in terms of continuum wave solutions to the time dependent Schrödinger equation for tunneling decay, yield identical numerical results [18–20]. This should not be confused with approaches where the Hamiltonian is separated into a part corresponding to a closed system and a part responsible for the decay which usually is treated to some order of perturbation theory, as in the work by Weisskopf and Wigner to describe the decay of an excited atom interacting with a quantized radiation field [21], that has become a standard procedure in some decay problems where perturbation theory may be justified.

The paper is organized as follows. Section 2 reviews briefly the formalism of resonant states. Section 3 analyzes some properties of the expansion of the decaying solution in terms of resonant states, and finally, Section 4 presents some concluding remarks.

2. Resonant state formalism

In this section we briefly recall the relevant points of the derivation of the decaying wave solution for a single particle confined initially, at \( t = 0 \), within the internal region of a real spherically symmetrical potential that vanishes beyond a distance, i.e., \( V(r) = 0 \) for \( r > a \). We choose the natural units \( \hbar = 2m = 1 \) and for simplicity of the description we refer to \( s \) waves. Therefore, the Hamiltonian to the system reads,

\[
H = -\frac{d^2}{dr^2} + V(r). \tag{1}
\]

Resonance states satisfy the time-dependent Schrödinger equation to the problem with outgoing boundary conditions, which imply complex energy eigenvalues [1–3],

\[
\left[ i \frac{\partial}{\partial t} - H \right] u_n(r, t) = 0, \tag{2}
\]

where,

\[
u_n(0, t) = 0, \quad u_n(r, t) = D_n(e^{i\alpha_n r}e^{-iE_n t})e^{i\beta_n r}e^{-\Gamma_n t/2}, \quad r \geq a. \tag{3}
\]

where we have used that \( \kappa_n = \alpha_n - i\beta_n \) and hence

\[
E_n = \kappa_n^2 = \mathcal{E}_n - i\Gamma_n/2, \tag{4}
\]

where \( \mathcal{E}_n = \alpha_n^2 - \beta_n^2 \) stands for the resonance energy of the decaying particle and \( \Gamma_n = 4\alpha_n\beta_n \) stands for the resonance or decaying width, which is related to the lifetime as, recalling that \( \hbar = 1 \), \( \tau_n = 1/\Gamma_n \).

Separation of variables in (2) yields [4],

\[
[\kappa_n^2 - H]u_n(r) = 0, \tag{5}
\]
where $u_n(r)$ satisfies outgoing (radiative) boundary conditions,

$$u_n(0) = 0, \quad \left[ \frac{d}{dr} u_n(r) \right]_{r=a} = i\kappa_n u_n(a).$$

Equation (3) represents an evolving outgoing wave times a term that grows exponentially with distance times another term that decreases exponentially with time. Clearly, the usual rules of normalization, orthogonality and completeness do not apply and, in addition, the corresponding probability density diminishes exponentially with time. It is therefore no surprising that this non-Hermitian approach has been considered as a simplified, phenomenological, and non fundamental description of the decay process, that in addition, violates the conservation of probability [22]. In spite of these apparently insuperable shortcomings work on an analytical description of the decay process has continued since the early work by Gamow. We will not discuss here the interesting historical developments on this subject. The present approach has evolved from considerations concerning the analytical properties of the Green’s function to the problem [16, 23, 24] as developed by the present author and his co-workers. See, for example, Refs. [18, 25, 26].

The solution to the time-dependent Schrödinger equation, as an initial value problem, may be written at time $t > 0$ in terms of the retarded Green’s function $g(r, r'; t)$ of the problem as [25],

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

where $\Psi(r, 0)$ stands for the arbitrary state initially 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 states. It is convenient to express the retarded time-dependent Green’s function in terms of the outgoing Green’s function $G^+(r, r'; k)$ of the problem. Both quantities are related by a Laplace transformation. The Bromwich contour in the $k$ complex plane corresponds to a hyperbolic contour along the first quadrant that may be deformed, since there are no bound states, to a contour that goes from $-\infty$ to $\infty$ along the real $k$ axis,

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

It is well known that for potentials that vanish exactly after a distance, the function $G^+(r, r'; k)$ has an infinite number of complex poles distributed on the $k$-plane in a well known manner [16]. Usually, except in special circumstances, these poles are simple and I assume that such is the case here. Since the potential is real, complex poles lie on the lower half of the $k$-plane distributed symmetrically with respect to the imaginary axis and there is an infinite number of them. Those located on the positive imaginary axis correspond to bound states and those on the imaginary axis to antibound states.

It is convenient to make use of the resonant expansion of the outgoing Green’s function [25],

$$G^+(r, r'; k) = \frac{1}{2k} \sum_{n=-\infty}^{\infty} \frac{u_n(r)u_n(r')}{k - \kappa_n}, \quad (r, r') \not\sim a$$

where the notation $(r, r') \not\sim a$ means that the point $r = r' = a$ is excluded in the above expansion (otherwise it diverges) and the set of functions $\{u_n(r)\}$ refer to the resonance states to the problem, which are obtained from the residues at the complex poles $\{\kappa_n\}$ of the outgoing Green’s function that also provide its normalization condition [24, 25],

$$\int_0^a u_n^2(r)dr + i\frac{u_n^2(a)}{2\kappa_n} = 1.$$
One should note that for $r' < a$ and $r \geq a$ one may write $G^+(r, r'; k)$ as \[18, 25\],
\[
G^+(r, r'; k) = G^+(r', a; k) e^{i k (r - a)}, \quad r' < a, \quad r \geq a.
\tag{11}
\]
The above expression permits to get a resonance expansion for $G^+(r, r'; k)$ which is valid along the external region of the interaction. On the other hand, it is easily shown by substitution of (11) into the equation that satisfies the outgoing Green’s function,
\[
[k^2 - H] G^+(r, r'; k) = \delta(r - r'),
\tag{12}
\]
that the representation of $G^+(r, r'; k)$ given by (9) satisfies the closure relation \[18\],
\[
\frac{1}{2} \sum_{n=-\infty}^{\infty} u_n(r) u_n(r') = \delta(r - r'), \quad (r, r')^\dagger \leq a,
\tag{13}
\]
and the sum rule,
\[
\sum_{n=-\infty}^{\infty} u_n(r) u_n(r') \kappa_n = 0, \quad (r, r')^\dagger \leq a
\tag{14}
\]
and also, after a simple algebraic manipulation, the additional sum rule \[18\],
\[
\sum_{n=-\infty}^{\infty} \frac{u_n(r) u_n(r')}{\kappa_n} = 0, \quad (r, r')^\dagger \leq a
\tag{15}
\]

The above results allows us to write the decaying time-dependent wave function as \[18, 25\],
\[
\Psi(r, t) = \sum_{n=-\infty}^{\infty} \begin{cases} 
C_n u_n(r) M(y_n), & r \leq a \\
C_n u_n(a) M(y_n), & r \geq a,
\end{cases}
\tag{16}
\]
where the coefficients $C_n$ are defined as,
\[
C_n = \int_0^a \Psi(r, 0) u_n(r) dr.
\tag{17}
\]
and the functions $M(y_n)$, the so named Moshinsky functions, are defined as \[25\]
\[
M(y_n) = \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{e^{i k (r - a)} e^{-ik^2 t}}{k - \kappa_n} dk = \frac{1}{2} e^{i (r - a)^2/4t} w(iy_n),
\tag{18}
\]
where
\[
y_n = e^{-i\pi/4} (1/4t)^{1/2} [(r - a) - 2\kappa_n t],
\tag{19}
\]
and the function $w(z) = \exp(-z^2) \text{erfc}(-iz)$ in (18) stands for the Faddeyeva–Terente’v or complex error function \[27\] for which there exist efficient computational tools to calculate it \[28\]. The argument $y_n^0$ of the functions $M(y_n^0)$ in (16) is that of $y_n$ given by (19) with $r = a$, namely,
\[
y_n^0 = -e^{-i\pi/4} \kappa_n t^{1/2}.
\tag{20}
\]

3. Properties of the decaying solution

Here, I discuss some properties of the expansion in resonant states of the decaying solution that involve the closure relation (13) and the sum rules given by (14) and (15). Some comments on the solutions along the internal and external interaction are also given.
3.1. Closure relation and quasi–probabilities

Assuming that the initial state $\Psi(r,0)$ is normalized to unity, it follows from the closure relation (13) that,

$$\text{Re} \left\{ \sum_{n=1}^{\infty} C_n \bar{C}_n \right\} = 1,$$

(21)

where $C_n$ is given by (17) and $\bar{C}_n$ reads,

$$\bar{C}_n = \int_0^a \Psi^*(r,0) u_n(r) dr.$$  

(22)

In writing (21) we have used the fact that the complex poles $\kappa_{-n}$ located on the third quadrant of the complex $k$-plane and corresponding resonant states $u_{-n}(r)$, fulfill from time reversal considerations [5,25],

$$\kappa_{-n} = -\kappa_n^*, \quad u_{-n}(r) = -u_n^*(r).$$  

(23)

Equation (21) shows that $\text{Re} \{C_n \bar{C}_n\}$ cannot be interpreted as a probability, since in general it is not a positive definite quantity. Nevertheless, one may see that it represents the ‘strength’ or ‘weight’ of the initial state in the corresponding resonant state. For example, for some $u_r(r)$, $\text{Re} C_r \bar{C}_r \approx 1$, and then (21) may hold with just one term. One might see the coefficients $\text{Re} \{C_n \bar{C}_n\}$ as some sort of quasi–probabilities. This point deserves further study.

3.2. Properties of the solution to the time-dependent Schrödinger equation

Although the derivation of the decaying solution in terms of the resonant states given by (16) is exact, it may be of interest to learn how it solves the time-dependent Schrödinger equation,

$$\left[ i \frac{\partial}{\partial t} - H \right] \Psi(r,t) = 0.$$  

(24)

Here I shall refer to the decaying solution along the internal region, given by the first expression in (16). Substitution of that expression in (24) may be written as,

$$i \sum_{n=-\infty}^{\infty} C_n u_n(r) \left[ \frac{\partial}{\partial t} M(y_n^\alpha) \right] - \sum_{n=-\infty}^{\infty} C_n M(y_n^\alpha) [Hu_n(r)] = 0.$$  

(25)

In order to solve (25) one may write,

$$\frac{\partial}{\partial t} M(y_n^\alpha) = \frac{\partial M(y_n^\alpha)}{\partial y_n^\alpha} \frac{\partial y_n^\alpha}{\partial t}.$$  

(26)

Then, using (18) with $r = a$, allows us to write,

$$M(y_n^\alpha) = \frac{1}{2} w(iy_n^\alpha),$$  

(27)

and hence one may write,

$$\frac{\partial M(y_n^\alpha)}{\partial y_n^\alpha} = \frac{i}{2} \frac{\partial w(iy_n^\alpha)}{\partial (iy_n^\alpha)},$$  

(28)

and, in view of (20),

$$\frac{\partial y_n^\alpha}{\partial t} = -\frac{1}{2} e^{-i\pi/4} \kappa_n \frac{1}{t^{1/2}}.$$  

(29)
Now, the partial derivative on right-hand side of (28), with \( z = iy_n^0 \), is given by Eq. (7.1.20) of ref. [27],
\[
\frac{dw(z)}{dz} = -2zw(z) + \frac{2i}{\sqrt{\pi}},
\]
and hence,
\[
\frac{\partial M(y_n^0)}{\partial y_n^0} = -2e^{-i\pi/4}\kappa_n t^{1/2}M(y_n^0) - \frac{1}{\sqrt{\pi}}.
\]
Substitution of (29) and (31) into (26) yields,
\[
\frac{\partial}{\partial t} M(y_n^0) = e^{-i\pi/2}\kappa_n^2 M(y_n^0) + \frac{1}{2\sqrt{\pi}}e^{-i\pi/4}\kappa_n \frac{1}{t^{1/2}}.
\]
One may then substitute (32) into (24) to write,
\[
\sum_{n=-\infty}^{\infty} C_n M(y_n^0) \left\{ [\kappa_n^2 - H]u_n(r) \right\} + \frac{e^{-i\pi/4}}{2\sqrt{\pi}} \left\{ \sum_{n=-\infty}^{\infty} C_n \kappa_n u_n(r) \right\} \frac{1}{t^{1/2}} = 0. \tag{33}
\]
One sees immediately, using (5), that the first term in (33) vanishes term by term whereas the vanishing of the second term follows from the sum rule (14), which involves the full resonant expansion. A similar procedure, though more involved mathematically, follows for the solution of the decaying solution for \( r \geq a \).

It might be of interest to write \( \Psi(r, t) \) for \( r < a \) as,
\[
\Psi(r, t) = \sum_{n=1}^{\infty} [C_n u_n(r) M(y_n^0) + \tilde{C}_n u_n^*(r) M(y_n^0)].
\]
Where, using (23), one may write the resonant expansion involving only the poles located on the fourth quadrant of the \( k \)-plane and make use of a property of the functions \( M(y_n^0) \) that establishes that,
\[
M(y_n^0) = \exp(-i\kappa_n^2 t) - M(-y_n^0),
\]
provided \( \pi/2 < \arg(y_n^0) < 3\pi/2 \) [25, 29]. This is in fact the case for resonance poles with \( \alpha_n > \beta_n \), the so called proper resonance poles located on the fourth quadrant of the \( k \)-plane. In such a case, the arguments of both \( M(-y_n^0) \) and \( M(y_n^0) \), satisfy \( -\pi/2 < \arg(y_n^0) < \pi/2 \), and hence, do not exhibit an exponential behavior. As a result, one may write (34) as the sum of exponential and nonexponential decaying terms,
\[
\Psi(r, t) = \Psi_e(r, t) + \Psi_{ne}(r, t), \quad r \leq a
\]
where \( \Psi_e(r, t) \) corresponds to the sum of exponential decaying terms
\[
\Psi_e(r, t) = \sum_{n=1}^{\infty} C_n u_n(r) e^{-i\kappa_n^2 t} e^{-\Gamma_n t/2}, \quad r \leq a
\]
and \( \Psi_{ne}(r, t) \) stands for the nonexponential contributions,
\[
\Psi_{ne}(r, t) = -\sum_{n=1}^{\infty} [C_n u_n(r) M(-y_n^0) - \tilde{C}_n u_n^*(r) M(y_n^0)], \quad r \leq a.
\]
It is easily verified by substitution of (37) into (24), that the purely exponential contribution satisfies (24) for each resonant term. In a similar fashion, this occurs also for the nonexponential
contributions (38), that involve terms proportional to $M(-y_0^n)$ and $M(y_0^n)$ and in addition reproduces the global term in (33) that vanishes due to the sum rule (14). It is worth mentioning that in a recent work [30] it is shown that the interference in the time domain of the exponential and nonexponential contributions of the decaying probability density provides a physical explanation for the exponential to nonexponential transition. This provides a non-Hermitian explanation for this transition, which in my view has not been provided provided using the standard formalism.

3.3. Nonexponential decay at long times

The long time behavior of $\Psi_{ne}(r,t)$ given by (38) follows from the asymptotic time behaviors of $M(-y_0^n)$ and $M(y_0^n)$. Using (27) one may use Eq. (7.1.23) of Ref. [27] to write

$$\Psi_{ne}(r,t) \approx -a \sum_{n=-\infty}^{\infty} \frac{C_n u_n(r)}{\kappa_n} \frac{1}{t^{1/2}} - b \sum_{n=-\infty}^{\infty} \frac{C_n u_n(r)}{\kappa_n^3} \frac{1}{t^{3/2}} + \cdots,$$

where $a = (i/2\sqrt{\pi i})$ and $b = (1/4\sqrt{\pi i})$. The relevant point here is that the term proportional to $1/t^{1/2}$, in view of the sum rule (15) cancels out exactly and therefore,

$$\Psi_{ne}(r,t) \approx -b \sum_{n=-\infty}^{\infty} \frac{C_n u_n(r)}{\kappa_n^3} \frac{1}{t^{3/2}} + \cdots.$$

The above result has also been obtained using the method of steepest descent [19].

3.4. Comments on the solutions along the internal and external interaction region

The decaying solution $\Psi(r,t)$ given by (16) may be studied as a function of the time $t$ for a fixed position $r$, along the internal or external interaction regions, or involving an integration along the internal region to calculate, in addition to the probability density, other quantities of interest as the survival and the non-escape probabilities [18,19,25]. Alternatively, the solution $\Psi(r,t)$ may be calculated for a fixed time $t_0$ as a function of the position $r$ both along the internal and external regions.

Along the internal region, $r \leq a$, given by the first equation in (16), $\Psi(r,t)$ exhibits how the probability density diminishes with time due to the decaying process, whereas along the external region, $r \geq a$, given by the second equation in (16), the solution describes the propagation of the decaying particle along the external region. An interesting feature of the above solutions is that along the internal region the analytical dependence on the position $r$ rests on the resonance functions $u_n(r)$ whereas the time dependence rests on the functions $M(y_n^0)$, as shows the argument $y_n^0$, given by (20). This might not be surprising since this is a common feature of solutions in the standard quantum formalism. However, along the external region, the corresponding solution involves, as shown by the second expression in (16), the resonance functions evaluated at $r = a$ whereas the propagating term, $M(y_n^0)$, exhibit both the dependence on position and on time, as shown by the corresponding argument $y_n$ given by (19). This is, indeed, a novel feature of the non-Hermitian solution. The above feature is crucial to exhibit the propagation of decaying probability density along the external region of the interaction at distinct values of time to show that the resonance expansion given by (16) fulfills unitarity [31].

4. Concluding remarks

The resonant-state formalism discussed here might be of particular interest for those pursuing 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.
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