PHYSICAL REVIEW
LETTERS

VOLUME 74 | 16 JANUARY 1995 | NUMBER 3

Resonant Spectra and the Time Evolution of the Survival and Nonescape Probabilities

G. García-Calderón, J. L. Mateos, and M. Moshinsky
Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000 México, D.F., México
(Received 12 May 1994)

The time evolution of quantum decay of an arbitrary state initially located within an interaction region of finite range is investigated. We compare the survival $S(t)$ and nonescape $P(t)$ probabilities. Our approach considers the full resonant spectra of the system using a novel representation of the time-dependent Green function. It is shown that, for an initial state near a resonance, $S(t)$ and $P(t)$ exhibit at long times a different behavior; not only the onset to a power law decay occurs at a different time, but also instead of the well known $S(t) \sim t^{-3}$ we obtain $P(t) \sim t^{-1}$.

PACS numbers: 03.65.–w, 73.40.Gk

The theoretical description of quantum decay refers to the time evolution of an initially confined arbitrary state $\psi(r, t = 0)$. Two notions that have been proposed to describe the time evolution of decay are the survival probability $S(t)$ of the initial state at a time t after the start of the process and the nonescape probability $P(t)$ to find the particle still confined at time t. Of the two notions the survival probability has been more widely used both in classical studies of decay [1] particularly regarding nonexponential contributions [2] and also in dynamical studies of quantum chaos [3]. Actually the survival and the nonescape probabilities correspond to two different definitions and types of phenomena [4]. For example, in the absence of decay, as in a closed region, the nonescape probability as a function of time is always unity, whereas the survival probability in general varies with time. Yet one finds rather disseminated the idea that the above two notions are equivalent.

In this Letter we address the question of how the resonant spectra of a system affects the time evolution of decay by using and comparing $S(t)$ and $P(t)$. In particular, we are interested in how the resonant spectra affects the nonexponential long time behavior. Our work has been to some extent motivated by the design and construction of artificial quantum structures [5] that may be used to investigate specific aspects of quantum mechanics.

Consider a single channel problem characterized by a potential of arbitrary shape $V(r)$ that vanishes after a distance, i.e., $V(r) = 0$ for $r > R$. One may solve the corresponding time-dependent Schrödinger equation in the radial variable r for s waves as an initial value problem. Denote by $\psi(r,0)$ the arbitrary state initially located within the internal region $0 \leq r \leq R$ at $t = 0$. Using the solution $\psi(r,t)$ at time t, the survival amplitude is defined as

$$A(t) = \int_0^R \psi^*(r,0)\psi(r,t)\,dr\,, \tag{1}$$

and $S(t) = |A(t)|^2$ is the probability of finding the state $\psi(r,t)$ at its initial value $\psi(r,0)$. On the other hand, the probability that the particle, described initially by $\psi(r,0)$, has not escaped away from the potential at time t is defined as

$$P(t) = \int_0^R \psi^*(r,t)\psi(r,t)\,dr\,. \tag{2}$$

The normalization of the initial state implies $S(0) = P(0) = 1$. The state $\psi(r,t)$ appearing in the above two definitions may be written in terms of the retarded time-dependent Green function as

$$\psi(r,t) = \int_0^R g(r,r';t)\psi(r',0)\,dr'\,. \tag{3}$$

$g(r,r';t)$ is the relevant quantity to describe the time evolution of the initial state. A convenient approach is to Laplace transform this quantity into the complex momentum k plane to exploit the analytical properties of the corresponding outgoing Green function $G^+(r,r';k)$,

$$g(r,r';t) = \frac{i}{2\pi}\int_{C_0} G^+(r,r';k)e^{-ik^2t}2k\,dk\,, \qquad (4)$$

where C_0 stands for the Bromwich contour and corresponds to an hyperbolic contour along the first quadrant on the k plane [6]. In the present approach, instead of the common practice of assuming the analytical properties of $G^+(r,r';k)$, we impose the condition, adequate on physical grounds, that the potential vanishes after a distance. As a consequence it can be rigorously proved that the propagator $G^+(r,r';k)$ may be extended analytically to the whole complex k plane where it has an infinite number of complex poles distributed in a well known manner [7]. As is well known these poles are the same as those of the S matrix of the system. At small energies the poles might be isolated, but at large energies they overlap with each other. The position of each pole in the complex k plane is a function of the parameters of the potential. We shall refer, for the sake of simplicity, to the case where only resonant poles are present. This is indeed a common situation in quantum structures.

The evaluation of $g(r,r';t)$ as an expansion in terms of the poles of $G^+(r,r';k)$ may be obtained by deforming appropriately the contour C_0 and using the theorem of residues. This leads to an expansion involving a sum of exponentially decaying terms, that arises from the poles on the fourth quadrant $k_p = a_p - ib_p$, the so-called proper resonant poles, plus an integral contribution along a path on the complex k plane [68], namely,

$$g(r,r';t) = \sum_{p=1}^{\infty} u_p(r)u_p(r')e^{-ik_p^2t} + \frac{i}{\pi}\int_{C_L} G^+(r,r';k)e^{-ik^2t}k\,dk\,. \qquad (5)$$

In the above expression, without loss of generality, we choose the path C_L as a straight line 45° off the real k axis that goes through the origin $k=0$ [6]. The functions $u_p(r)$ in Eq. (5) correspond to the resonant states of the system. They may be seen as solutions of the radial Schrödinger equation of the problem obeying outgoing boundary conditions [9]. This leads to complex eigenvalues, $E_p = k_p^2 = \epsilon_p - i\Gamma_p/2$, where ϵ_p represents the position of the resonance and Γ_p the corresponding width. The states $u_p(r)$ may also be defined as the residues at the complex poles k_p of $G^+(r,r';k)$. This provides its normalization condition [6,10]. The above definitions for the states $u_p(r)$ apply also to the states u_{-p} associated with the poles k_{-p} located on the third quadrant of the k plane. It follows from time reversal invariance that $k_{-p} = -k_p^*$ and $u_{-p}(r) = u_p^*(r)$. One may use Eqs. (3) and (5) into Eq. (1) to write the survival amplitude as a resonant sum plus an integral term. However, it is not a simple task to evaluate the integral term except at long times compared with the lifetime of the system, where it gives the well known $t^{-3/2}$ behavior [1].

It turns out, however, that if the quantities of interest are defined along the internal region of the interaction, as $S(t)$ and $P(t)$, then it is possible to show that the integral term in Eq. (5) may be written also as a sum over resonant terms. This leads to a representation of the time-dependent Green function as a purely discrete resonant expansion that describes both the exponential and nonexponential contributions to the time evolution of decay. The key point is to realize that $G^+(r,r';k)$, for any value of k on the complex k plane, may be expanded along the internal region of the interaction as an infinite sum over the full set of resonant states of the problem [10],

$$G^+(r,r';k) = \sum_{n=-\infty}^{\infty}\frac{u_n(r)u_n(r')}{2k_n(k-k_n)}\,, \qquad (r,r') < R\,. \quad (6)$$

The above expansion is obtained using Cauchy integral theorem, and its validity, provided $(r,r') < R$, is based on the rigorous proof that $G^+(r,r';k) \to 0$ as $|k| \to \infty$ along all directions of the complex k plane [11]. It can also be proved that Eq. (6) implies the relations [10]

$$\sum_{n=-\infty}^{\infty}\frac{u_n(r)u_n(r')}{k_n} = 0, \qquad (r,r') < R\,, \qquad (7)$$

$$\frac{1}{2}\sum_{n=-\infty}^{\infty} u_n(r)u_n(r') = \delta(r-r'), \qquad (r,r') < R\,. \quad (8)$$

Substituting Eq. (6) into the right hand side of Eq. (5) leads to an expansion over the full set of resonant states that may be written as [12]

$$g(r,r';t) = \sum_{n=-\infty}^{\infty} u_n(r)u_n(r')M(k_n,t), \qquad (r,r') < R, \qquad (9)$$

where the functions $M(k_n,t)$ are defined as [13]

$$M(k_n,t) \equiv \frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{e^{-ik^2t}}{k-k_n}\,dk = \frac{1}{2}e^{u^2}\operatorname{erfc}(u)\,, \qquad (10)$$

with $u = -\exp(-i\pi/4)k_nt^{1/2}$. The function $M(k_n,t)$ is a particular case of a type of integrals that appear in the description of transient effects, see Eq. (52) of Ref. [14]. Since $M(k_n,0) = 1/2$, it is immediately apparent that for $t \to 0$ Eq. (9) goes into Eq. (8). Note that in deriving Eq. (9) there appear the functions $M(-k_n,t)$ and $M(-k_n^*,t)$ that are defined as Eq. (10) but with the argument u given, respectively, by $u = \exp(-i\pi/4)k_nt^{1/2}$ and $u = \exp(-i\pi/4)k_n^*t^{1/2}$.

Substitution of Eq. (9) into Eq. (1), using Eq. (3) gives for the survival amplitude

$$A(t) = \sum_{n=-\infty}^{\infty} C_n\bar{C}_nM(k_n,t)\,. \qquad (11)$$

Here n runs through the resonant poles on the third and fourth quadrants of the k plane, and the coefficients C_n and $\bar{C}_n$ are defined as

$$C_n = \int_0^R \psi(r,0)u_n(r)\,dr, \qquad \bar{C}_n = \int_0^R \psi^*(r,0)u_n(r)\,dr. \tag{12}$$

Note that as long ago as 1951, one of the authors (M. M.) had given an exact expression of $A(t)$ for the one-level case, i.e., when only $k_{\pm 1} \neq 0$; see Eq. (27b) of Ref. [14]. Using Eq. (11) the survival probability, $S(t) = |A(t)|^2$, may be written as

$$S(t) = \sum_{n=-\infty}^{\infty} \sum_{\ell=-\infty}^{\infty} C_n \bar{C}_n C_\ell^* \bar{C}_\ell^* M(k_n,t) M^*(k_\ell,t). \tag{13}$$

Similarly the nonescape probability, by substitution of (9) into (3), using (12), reads

$$P(t) = \sum_{n=-\infty}^{\infty} \sum_{\ell=-\infty}^{\infty} C_n C_\ell^* I_{n\ell} M(k_n,t) M^*(k_\ell,t). \tag{14}$$

In the above equation $I_{n\ell}$ is defined by

$$I_{n\ell} = \int_0^R u_\ell^*(r) u_n(r)\,dr. \tag{15}$$

Notice that $S(t)$ and $P(t)$ are very similar. The integrals $I_{n\ell}$ appearing in $P(t)$ replace the product of coefficients $\bar{C}_n \bar{C}_\ell^*$ that occur in $S(t)$. Actually the coefficients (12) obey some useful relations. Multiply both Eqs. (7) and (8) by $\psi(r,0)$ and $\psi^*(r',0)$ and integrate the result from $r = 0$ to $r = R$. We obtain

$$\sum_{n=-\infty}^{\infty} \frac{C_n \bar{C}_n}{k_n} = 0, \tag{16}$$

$$\frac{1}{2} \sum_{n=-\infty}^{\infty} C_n \bar{C}_n = 1. \tag{17}$$

Equations (9), (11), (13), and (14) are given in terms of M functions, and hence their exponential and nonexponential behavior is not exhibited explicitly. This can be achieved by using the symmetry relations between the poles on the third and fourth quadrants mentioned before, to write the sums only over the poles on the fourth quadrant, and using the relation [12,13]

$$M(k_p,t) = e^{-ik_p^2 t} - M(-k_p,t). \tag{18}$$

For example, if the initial state is close to a sharp isolated resonant state, say $u_s(r)$, then it may be seen that $I_{ss} \approx 1$ and from (17), that $\mathrm{Re}\, C_s \bar{C}_s \approx 1$. If, in addition, Γ_s is the longest lifetime, then the dominant term in Eqs. (13) and (14) is $n = s$, and hence, ignoring the nonexponential contributions, one obtains the well known exponential decay law, $S(t) = P(t) = e^{-\Gamma_s t}$.

Let us now turn to the analysis of the long time behavior. From Eq. (18) one sees that asymptotically the relevant terms are of the type $M(-k_n,t)$ where k_n stands for either k_p or k_p^*. From the definition (10) using the asymptotic expansion of $\exp(u^2)\mathrm{erfc}(u)$ one gets [12,13]

$$M(-k_n,t) \approx \alpha\left(\frac{1}{k_n t^{1/2}}\right) - \beta\left(\frac{1}{k_n^3 t^{3/2}}\right) + \cdots, \tag{19}$$

where $\alpha = i/2(\pi i)^{1/2}$ and $\beta = 1/4(\pi i)^{1/2}$. Substitution of Eq. (19) into (11), in view of (18), allows us to write $A(t)$ as a sum over proper poles involving exponentially decaying terms plus sums of terms that are like inverse powers of time. One may see, however, that the coefficient proportional to $t^{-1/2}$ is identical to Eq. (16), and therefore it cancels out exactly. Consequently, the survival amplitude reads

$$A(t) \approx \sum_{p=1}^{\infty}\left(C_p \bar{C}_p e^{-ik_p^2 t} - 2i\beta\, \mathrm{Im}\left(\frac{C_p \bar{C}_p}{k_p^3}\right)\frac{1}{t^{3/2}} + \cdots\right). \tag{20}$$

The above equation exhibits the crossover from exponential to a power law behavior. Using (20) one sees that the survival probability behaves at long times as t^{-3}.

Let us now consider the long time behavior of the nonescape probability. One sees from Eq. (9) into Eq. (2) for $P(t)$ that the resonant expansion of $g(r,r';t)$ is coupled through the integration over r with that of $g^*(r,r';t)$. This gives origin to the integrals $I_{n\ell}$ defined by (15). Hence when the asymptotic expansion of the M functions (19) is introduced into (14), the leading contribution is proportional to t^{-1} and includes terms of the type

$$\sum_r^{\infty} \sum_s^{\infty} \left(\frac{C_r^* C_s I_{rs}}{k_r^* k_s}\right) \frac{1}{t} \tag{21}$$

that are different from (16) and hence do not cancel. In other words, asymptotically, $P(t) \sim t^{-1}$. Hence $S(t)$ and $P(t)$ behave differently at long times.

We consider, as a numerical example of our results, a comparison between the survival and nonescape probabilities for the case of the delta-shell potential $V(r) = b\delta(r - R)$, with b the intensity, and the initially confined state at $t = 0$, $\psi(r,0) = 2^{1/2}\sin(q\pi/R)r$. The units are $\hbar = 2m = R = 1$, and the value of $b = 200$. One may obtain the set of poles $\{k_n\}$ and resonant states $\{u_n(r)\}$ along the region $0 < r < 1$ of the problem [12,13] to evaluate $S(t)$ and $P(t)$ using Eqs. (13) and (14). Figure 1 shows a plot, using 500 poles, of both $\ln S(t)$ (solid line) and $\ln P(t)$ (dashed line) for an initial state with $q = 1$, which is situated very near the first resonance, as a function of time t in units of the lifetime $1/\Gamma_1$. One sees that along the exponentially decaying region both quantities coincide for a number of lifetimes. However, eventually the nonescape probability goes into the power law t^{-1} behavior. About 20 lifetimes later, the survival amplitude starts oscillating before going into the power law t^{-3} behavior. The oscillations are not observed in $P(t)$ because of the overlap integrals (15). The early onset of $P(t)$ to a power law compared with that of $S(t)$ is a general result and might be relevant in attempts to measure nonexponential contributions to decay [15].

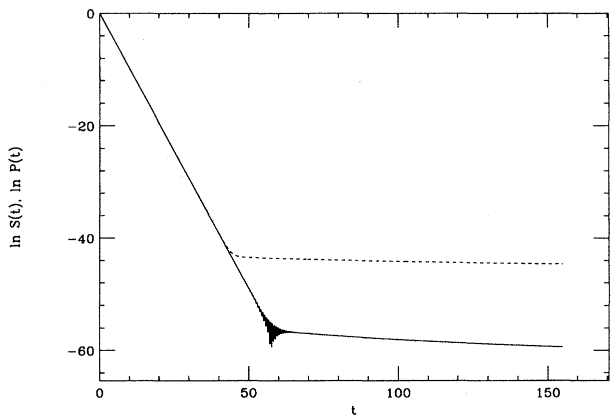

FIG. 1. Plot of $\ln S(t)$ and $\ln P(t)$ as a function of time for an initial state very near the first resonance of the delta-shell potential as described in the text.

Figure 2 shows a case where the initial state is near the second resonant state, i.e., $q = 2$. One first observes that $S(t)$ and $P(t)$ decay exponentially at the beginning with slope Γ_2 and then split. However, they continue to decay exponentially, now with slope Γ_1, to finally suffer a transition to a power law behavior, $S(t) \sim t^{-3}$ and $P(t) \sim t^{-1}$. Notice that the onset to the different regimes occurs at different time for both quantities. More generally, both for $S(t)$ and $P(t)$, any excited state ($q \neq 1$) goes to the ground state ($q = 1$), before the crossover to a power law decay. A more detailed discussion of these behaviors, including initial states far from resonance, will be considered elsewhere [16].

In summary, we have derived representations for the survival and the nonescape probabilities in terms of the full resonant spectra of the system for an arbitrary initially confined state, that are valid at all times. We have compared the above quantities and showed that at long times they obey a different power law decay. We believe that our results are relevant to investigations on the deviation from the exponential decay law and also in studies of the time evolution of initially confined states in novel quantum structures.

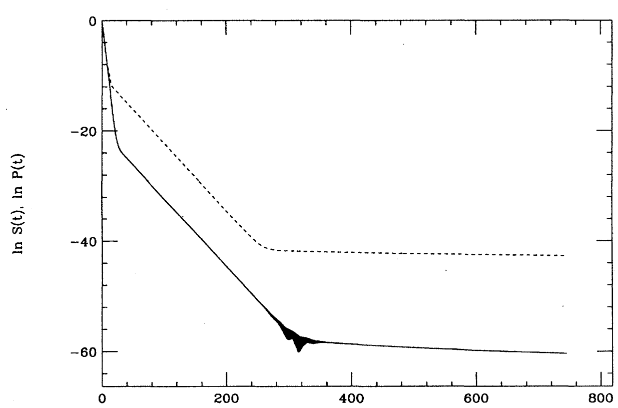

FIG. 2. Plot of $\ln S(t)$ and $\ln P(t)$ as a function of time for an initial state very near the second resonance of the delta-shell potential as described in the text.

This work was partially supported by DGAPA-UNAM No. IN-101693. We thank K. W. McVoy for useful discussions.

[1] M. L. Goldberger and K. M. Watson, *Collision Theory* (John Wiley & Sons, Inc., New York, 1964), Chap. 8.
[2] Nonexponential contributions to decay were first discussed by L. A. Khalfin, Zh. Eksp. Teor. Fiz. **33**, 1371 (1957) [Sov. Phys. JETP **6**, 1053 (1958)]. See, however, Ref. [13], where the exact solution of the time evolution of decay due to a single level of the S matrix includes already nonexponential contributions. See also R. G. Newton, Ann. Phys. (N.Y.) **14**, 333 (1961); A. Peres, Ann. Phys. (N.Y.) **129**, 33 (1980), and references therein.
[3] See, for example, E. J. Heller, in *Chaos and Quantum Physics,* edited by M. J. Giannoni, A. Voros, and J. Zinn-Justin (North-Holland, Amsterdam, 1991), and references therein.
[4] R. B. Frey and E. Thiele, J. Chem. Phys. **48**, 3240 (1968).
[5] See, for example, *Transport Phenomena in Mesoscopic systems,* edited by H. Fukuyama and T. Ando (Springer-Verlag, Berlin, 1992).
[6] G. García-Calderón and R. E. Peierls, Nucl. Phys. **A265**, 441 (1976).
[7] R. G. Newton, *Scattering Theory of Waves and Particles* (Springer-Verlag, Berlin, 1982), Chap. 12.
[8] E. C. G. Sudarshan, C. B. Chiu, and V. Gorini, Phys. Rev. D **18**, 2914 (1978).
[9] G. Gamow, Z. Phys. **51**, 204 (1928).
[10] See, for example, R. More, Phys. Rev. A **4**, 1782 (1971); G. García-Calderón, Lett. Nuovo Cimento **33**, 253 (1982).
[11] G. García-Calderón and M. Berrondo, Lett. Nuovo Cimento **26**, 562 (1979).
[12] G. García-Calderón, in *Symmetries in Physics,* edited by A. Frank and K. B. Wolf (Springer-Verlag, Berlin, 1992), p. 252.
[13] G. García-Calderón, G. Loyola, and M. Moshinsky, in *Symmetries in Physics,* edited by A. Frank and K. B. Wolf (Springer-Verlag, Berlin, 1992), p. 273.
[14] M. Moshinsky, Phys. Rev. **84**, 525 (1951).
[15] E. B. Norman, S. B. Gazes, S. G. Crane, and D. A. Bennett, Phys. Rev. Lett. **60**, 2246 (1988).
[16] G. García-Calderón, J. L. Mateos, and M. Moshinsky (unpublished).