Survival and Nonescape Probabilities for Resonant and Nonresonant Decay

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In this paper we study the time evolution of the decay process for a particle confined initially in a finite region of space, extending our analysis given recently (*Phys. Rev. Lett.* **74**, 337 (1995)). For this purpose, we solve exactly the time-dependent Schrödinger equation for a finite-range potential. We calculate and compare two quantities: (i) the survival probability $S(t)$, i.e., the probability that the particle is in the initial state after a time t; and (ii) the nonescape probability $P(t)$, i.e., the probability that the particle remains confined inside the potential region after a time t. We analyze in detail the resonant and nonresonant decay. In the former case, after a very short time $S(t)$ and $P(t)$ decay exponentially, but for very long times they decay as a power law, albeit with different exponents. For the nonresonant case we obtain that both quantities differ initially. However, independently of the resonant and nonresonant character of the initial state we always find a transition to the ground state of the system which indicates a process of "loss of memory" in the decay.   © 1996 Academic Press, Inc.

I. INTRODUCTION

In a recent publication [1], we study the time evolution of the decay process in quantum mechanics for a particle initially confined in a finite region of space. We were able to solve exactly the time-dependent Schrödinger equation for a finite range central potential $V(r)$ by considering the full resonant spectra of the system using a novel representation of the time-dependent Green function in terms of resonant states.

Once we obtain the wave function $\psi(r, t)$ for our problem we calculate and compare two quantities: (i) the survival probability $S(t)$, that is, the probability that the particle is in the initial state after a time t; (ii) the nonescape probability $P(t)$, defined as the probability that the particle remains confined inside the potential region after a time t. Of the two notions the survival probability has been more widely used, presumably because it can be manipulated in a more abstract way, without referring to an initially confining region of space for the decaying particle. One finds that the notion of survival probability has been commonly used in studies of quantum decay [2] and also in dynamical studies of quantum chaos [3].

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Actually the survival and nonescape probabilities correspond to two different notions [4, 5]. For instance, a particle can leave the initial state $\psi(r, 0)$ while remaining inside the potential. In such a case $S(t)$ varies with time while $P(t)$ is always unity.

In this paper we will analyze in detail resonant and nonresonant decay. The former refers to the situation where the energy of the initial state is close to one of the resonances of the system. This case was considered in Ref. [1] and here we extend the discussion also to the nonresonant decay, that is the case where the energy of the initial state is arbitrary.

A comparison between the survival and nonescape probabilities might be of particular interest in connection with the problem of the nonexponential contributions to the time evolution of quantum decay [2, 6, 7]; in threshold effects in photoionzation in atomic physics [8] and in radioactive decay of nuclei [9, 10]; in one dimensional quantum tunneling [11]; in tunneling dynamics of squeezed states [12], and in studies of the time evolution of chaotic quantum systems [3, 13].

A novel feature of our approach is that the exponential and nonexponential contributions to the time evolution of decay are presented in terms of the full set of complex poles and resonant states associated with the outgoing Green function of the system. The description covers the full time interval from $0 \leqslant t < \infty$ and, in particular, it allows us to study the effect of the far away resonances on the time evolution properties of the system.

We shall discuss the above notions for a symmetrical potential $V(r)$ as shown in Fig. 1, and for simplicity we shall restrict ourselves to s-waves. A first question is whether $S(t)$ and $P(t)$ can be obtained in an analytic and explicit fashion, and the answer is yes, if $\psi(r, 0)$ is available in an explicit analytic form. This discussion will be carried out for arbitrary $V(r)$ and $\psi(r, 0)$ in Section II using an approach by
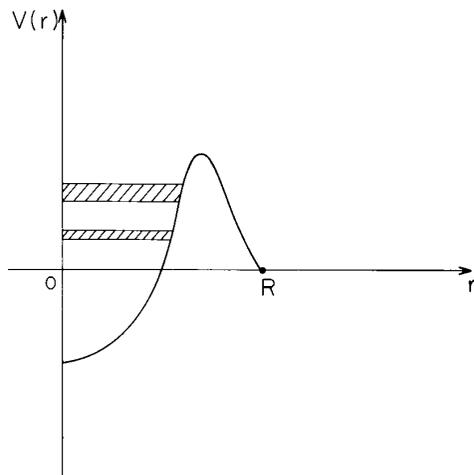

FIG. 1. Short range potential $V(r)$ between $r = 0$ and $r = R$. The dashed areas indicate schematically two resonant states, which are centered around an energy E_i and have a width Γ_i.

García-Calderón [6]. First we provide the stationary Green function of the problem as an expansion involving the resonant states and complex poles of the problem and then, with the help of the inverse Laplace transform, get the time-dependent Green function as an infinite sum of terms. Each term consists of coefficients involving the overlap of the initial state and the corresponding resonant state, multiplied by a function (introduced long ago by Moshinsky [14]) that depends on the complex energy and the time.

Once the probabilities of survival and nonescape are explicitly determined comes the interesting question of discussing their behavior and then comparing $S(t)$ and $P(t)$ for different times. For the resonant case we obtain that, after a very short time, both quantities decay exponentially and coincide with each other; however, for the nonresonant case in general differ considerably. Independently of the resonant or nonresonant character of the initial state we always find a crossover to the ground state of the system which indicates a process of "loss of memory." We will also derive with more detail the main result of Ref. [1], namely, that for long times, $S(t)$ and $P(t)$ behave in a different way: $P(t) \sim t^{-1}$ while $S(t)$ obeys the well known power law decay $\sim t^{-3}$.

To illustrate the approach it is convenient to consider a specific example and thus in Section III we take the case of the delta-function potential, $V(r) = b\delta(r - R)$, and a simple analytical expression for the initial state $\psi(r, 0) = \beta(\kappa) \sin \kappa r$. We shall in particular analyze the case where the strength of the δ-function potential is very large, i.e., in our units $b \gg 1$, because then one can derive an approximate analytical expression for the poles of the Green function. This will allow us to discuss in Section IV what happens to $S(t)$ and $P(t)$ when the initial state is near resonance and compare it with the situation when the initial state is off-resonance. Another aspect of interest is the behavior of $S(t)$ and $P(t)$ at different times and in particular the change from exponential to a power law behaviour which we shall also illustrate numerically.

II. DETERMINATION OF THE SURVIVAL AND NONESCAPE PROBABILITIES

The situation that we may confront then is that of a potential $V(r)$, as drawn in Fig. 1, that terminates at $r = R$. Our initial normalized wave function is restricted to the interval $0 \leqslant r \leqslant R$. We can then solve the time-dependent radial Schrödinger equation with the potential $V(r)$ and the initial condition mentioned above at $t = 0$ and denote the solution by $\psi(r, t)$. With the help of the latter we can define the survival amplitude $A(t)$ [2, 4, 5] as

$$A(t) = \int_0^R \psi^*(r, 0) \, \psi(r, t) \, dr \tag{2.1}$$

so that $S(t) = |A(t)|^2$ is the probability of finding at time t the state $\psi(r, t)$ at its initial value $\psi(r, 0)$, that is,

$$S(t) = \left| \int_0^R \psi^*(r, 0)\, \psi(r, t)\, dr \right|^2. \tag{2.2}$$

On the other hand, the probability that the particle does not escape from the potential is

$$P(t) = \int_0^R \psi^*(r, t)\, \psi(r, t)\, dr, \tag{2.3}$$

as the wave function $\psi(r, t)$ remains normalized if that was the case for its original value $\psi(r, 0)$. Thus the probability that the particle escapes is $1 - P(t)$. We shall denote $P(t)$ as the nonescape probability.

To derive a procedure for determining $S(t)$ and $P(t)$, we require first to find a solution of the time-dependent Schrödinger equation for a potential that vanishes beyond a distance, i.e., $V(r) = 0$; $r > R$ (Fig. 1), and the initial condition $\psi(r, 0)$. It is convenient first to determine the time dependent Green function, which we denote by $g(r, r', t)$ and which satisfies the equation

$$\left[-\frac{\partial^2}{\partial r^2} + V(r) \right] g(r, r', t) = i\frac{\partial}{\partial t}\, g(r, r', t), \tag{2.4}$$

with the initial condition

$$g(r, r', 0) = \delta(r - r'), \tag{2.5}$$

where we take $h = 2M = 1$ and, hence, $E = k^2$.

We proceed then to find the Laplace transform of this Green function which we denote by $\bar{g}(r, r'; s)$ given by

$$\bar{g}(r, r'; s) = \int_0^\infty g(r, r', t)e^{-st}\, dt. \tag{2.6}$$

Instead of the complex variable s it is convenient to introduce the variable k obeying,

$$s = (-ik^2), \qquad k \equiv (is)^{1/2}, \tag{2.7}$$

and to define the outgoing Green function $G^+(r, r'; k)$, which is used normally in the literature [15] through,
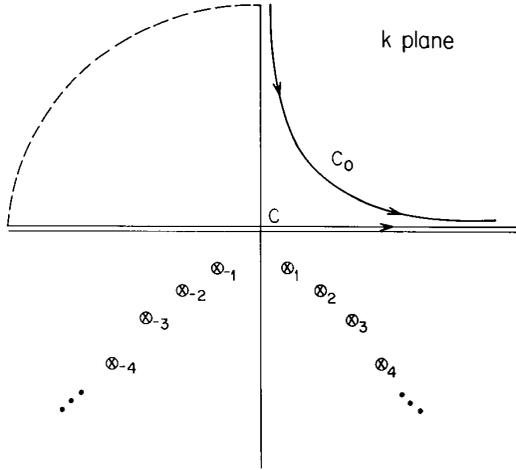
$$G^+(r, r'; k) \equiv i\bar{g}(r, r'; s). \tag{2.8}$$

FIG. 2. The Bromwhich contour C_0 in the k-plane for the integral given by Eq. (2.10), which can be modified to the real axis C, due to the factor $\exp(-ik^2t)$, which forces the integral to vanish on the portion of the circle indicated by the dashed line. The complex poles of the Green function (2.11) found on the lower half k-plane are also indicated.

Applying then the transform to both sides of Eq. (2.4) we obtain, using Eq. (2.8),

$$\left[\frac{\partial^2}{\partial r^2} + k^2 - V(r)\right] G^+(r, r'; k) = \delta(r - r').\tag{2.9}$$

Once the Laplace transform (26) is determined, we can get $g(r, r', t)$ by the inverse Laplace transform over the Bromwich contour but, in terms of the variable k, the integral is over the hyperbolic contour C_0 of Fig. 2 and we obtain [6, 16]

$$g(r, r', t) = \frac{i}{2\pi} \int_{C_0} G^+(r, r'; k)\, e^{-ik^2t} 2k\, dk.\tag{2.10}$$

Thus our first objective will be to obtain $G^+(r, r'; k)$.

A. Determination of $G^+(r, r'; k)$

Turning our attention back to Eq. (2.4) we note that for $r \neq r'$, $G^+(r, r'; k)$ satisfies an homogeneous ordinary differential equation, namely the Schrödinger equation of the problem. It is well known that $G^+(r, r'; k)$ may be written as [15],

$$G^+(r, r'; k) = -\frac{\phi(k, r_<)\, f(k, r_>)}{W(k)},\tag{2.11}$$

where $r_<$ indicates the smaller of r and r' and $r_>$, the larger. The function $\phi(k, r)$ stands for the regular solution of the Schrödinger equation of the problem with boundary conditions at the origin,

$$\phi((k, 0) = 0, \qquad [\partial\phi(k, r)/\partial r]_{r=0} = 1, \tag{2.12}$$

and the function $f(k, r)$ is irregular at the origin and is defined by the condition that for $r > R$ (since the potential vanishes beyond the distance R), it behaves as $\exp(ikr)$, namely an outgoing wave, which implies that for $r = R$ it satisfies,

$$f(k, R) = e^{ikR}, \qquad [\partial f(k, r)/\partial r]_{r=R} = ike^{ikR}, \tag{2.13}$$

which also defines it completely. The function $W(k)$ represents the Wronskian,

$$W(k) = \phi(k, r)\frac{\partial f(k, r)}{\partial r} - f(k, r)\frac{\partial \phi(k, r)}{\partial r}. \tag{2.14}$$

It is well known [15] that for a finite range interaction the outgoing Green function $G^+(r, r'; k)$, as a function of k, can be extended analytically to the whole complex k-plane, where it has an infinite number of poles that arise from the zeros of the Wronskian (2.14) and are distributed in a well-known manner [15, 17]. Purely imaginary poles on the upper half k-plane correspond to the bound states of the problem, whereas purely imaginary poles seated on the lower half k-plane correspond to antibound states. On the other hand, complex poles are only found on the lower half k-plane. To each complex pole at $k_n = a_n - ib_n$, with a_n, $b_n > 0$ there corresponds, due to time reversal invariance, a complex pole k_{-n} situated symmetrically with respect to the imaginary axis, i.e., $k_{-n} = -k_n^*$. In the examples that we shall discuss later, we shall assume potentials with no attractive part so they have no bound states, and, thus, all the poles of $G^+(r, r'; k)$ will be in the lower half of the complex k-plane. Hence our analysis is restricted to resonant states.

As shown below the complex poles of the outgoing Green function are related to the resonant states of the system. Resonant states may be defined as solutions of the Schrödinger equation of the problem [18, 19, 16]

$$\frac{d^2u_n(r)}{dr^2} + [k_n^2 - V(r)]u_n(r) = 0, \tag{2.15}$$

that obey the usual boundary condition at the origin,

$$u_n(0) = 0, \tag{2.16}$$

and at distances, $r \geqslant R$, describe a situation where there are no incident particles, namely, $u_n(r) \propto \exp(ik_nr)$, and hence they satisfy the outgoing boundary condition,

$$\left[\frac{du_n(r)}{dr}\right]_{r=R_-} = ik_nu_n(R). \tag{2.17}$$

Gamow [18] showed that the outgoing boundary condition (2.17) implies that the energy eigenvalues of the problem are necesarily complex, namely, $k_n^2 = E_n = \varepsilon_n - i\Gamma_n/2$, where ε_n stands for the position of the resonance and Γ_n refers to the corresponding width. The above boundary conditions also provide the bound and antibound solutions corresponding, respectively, to imaginary positive, $k_n = i\gamma_m$, and imaginary negative, $k_n = -i\delta_n$, values of k_n, where both γ_n and δ_n are real. The above complex eigenvalues correspond precisely to the complex poles of the outgoing Green function of the problem $G^+(r, r'; k)$. Moreover, it turns out that resonant states may also be defined as the residues at the complex poles k_n of $G^+(r, r'; k)$ [20]. Here we follow García-Calderón [6] to write,

$$R(r, r', k_n) = \lim_{k \to k_n} \{(k - k_n) G^+(r, r', k)\} = \frac{u_n(r) u_n(r')}{2k_n}, \tag{2.18}$$

provided the resonant states normalize according to

$$\int_0^R u_n^2(r) \, dr + \frac{i}{2k_n} u_n^2(R) = 1. \tag{2.19}$$

Let us now consider the integral [6]

$$\frac{1}{2\pi i} \int_{C'} \frac{G^+(r, r'; z)}{z - k} \, dz = 0, \tag{2.20}$$

which is taken over the contour C' of Fig. 3, consisting of one large cycle, whose radius will eventually go to ∞, and small circles surrounding all the poles of
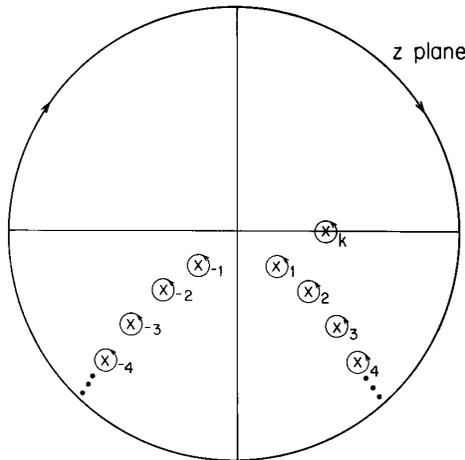

FIG. 3. The contour C' in the z-plane for the integral given by Eq. (2.20), consisting of one large circle and small circles surrounding all the poles of $G^+(r, r', z)$ as well as $z = k$.

$G^+(r, r'; z)$ in the z plane as well as the point where $z = k$. As the integrand is analytic inside this contour the integral vanishes, as indicated on the right-hand side of (2.20).

For the large circle, when $|z| \to \infty$, we can, in the upper half I_+ of the z plane, essentially disregard the potential $V(r)$ in Eq. (2.9) and, thus, $G^+(r, r'; z)$, obtained from (2.11), when we replace k by z, becomes

$$z^{-1}\{e^{iz(r+r')} - e^{iz(r'-r)}\}, \qquad \text{if} \quad 0 \leqslant r \leqslant r' \leqslant R, \qquad (2.21a)$$

$$z^{-1}\{e^{iz(r+r')} - e^{iz(r-r')}\}, \qquad \text{if} \quad 0 \leqslant r' \leqslant r \leqslant R, \qquad (2.21b)$$

which clearly vanishes, at least as $|z|^{-1}$ when $z = x + iy$, with $y > 0$. For the lower half I_- of the z plane, and the real axis, the analysis is more complicated. García-Calderón and Berrondo [21] have shown though, using appropriate forms of the Born approximation, that $G^+(r, r'; z)$ vanishes there exponentially, provided $(r, r') < R$. Thus there is no contribution from the large circle in Fig. 3 and, considering the contributions from all the small circles, including the one around $z = k$, one obtains [6, 22–25]

$$G^+(r, r'; k) = \sum_{n=-\infty}^{\infty} \frac{u_n(r) u_n(r')}{2k_n(k - k_n)}; \qquad (r, r') < R. \qquad (2.22)$$

Substitution of Eq. (2.22) into Eq. (2.9) yields, after straightforward algebra, the relations [6, 25]

$$\sum_{n=-\infty}^{\infty} \frac{u_n(r) u_n(r')}{k_n} = 0; \qquad (r, r') < R, \qquad (2.23)$$

and

$$\frac{1}{2} \sum_{n=-\infty}^{\infty} u_n(r) u_n(r') = \delta(r - r'); \qquad (r, r') < R. \qquad (2.24)$$

Equations (2.24) have been derived also following an expansion of $G^+(r, r'; k)$ in terms of inverse powers of k [22, 23]. Notice that

$$\frac{1}{2k_n(k - k_n)} \equiv \frac{1}{2k} \left[\frac{1}{k - k_n} + \frac{1}{k_n} \right], \qquad (2.25)$$

so then using Eq. (2.23) one may write Eq. (2.22) as

$$G^+(r, r', k) = \frac{1}{2k} \sum_{n=-\infty}^{\infty} \frac{u_n(r) u_n(r')}{(k - k_n)}; \qquad (r, r') < R. \qquad (2.26)$$

B. *Determination of $g(r, r', t)$*

One way to determine $g(r, r', t)$ is deforming the contour C_0 of Fig. 2 to exploit the analytical properties of $G^+(r, r'; k)$ using the theorem of residues. In this form

one may obtain expansions involving a sum of exponentially decaying terms plus an integral contribution along a certain path of the complex k-plane [16, 26]. If the potential vanishes beyond a distance and the notions of interest are defined within the potential region, as happens for the survival and nonescape probabilities defined by Eqs. (2.2) and (2.3), we can proceed as follows. First we deform the contour C_0 to the contour C as shown in Fig. 2. This can be easily done because $\exp(-ik^2t)$ converges as k increases in the upper left quadrant of the k-plane. Since we have assumed absence of bound states we then may write Eq. (2.10) as,

$$g(r, r', t) = \frac{i}{2\pi} \int_{-\infty}^{\infty} G^+(r, r'; k) \, e^{-ik^2t} 2k \, dk. \tag{2.27}$$

We can then substitute Eq. (2.26) into Eq. (2.27) to obtain an expansion of $g(r, r', t)$ in terms of the resonant states of the problem. The only integral we need to determine is

$$\frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-ik^2t}}{k - k_n} \, dk. \tag{2.28}$$

Moshinsky [29] has discussed the above type of integral. It appears in the description of transient effects in time dependent problems in quantum mechanics [30, 31] and it may be denoted as

$$M(k_n, t) \equiv \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-ik^2t}}{k - k_n} \, dk = \frac{1}{2} e^{u^2} \operatorname{erfc}(u), \tag{2.29}$$

where

$$u = -\exp(-i\pi/4) \, k_n \, t^{1/2}. \tag{2.30}$$

Thus the time-dependent Green function $g(r, r', t)$ takes the form first derived by García-Calderón [6],

$$g(r, r', t) = \sum_{n=-\infty}^{\infty} u_n(r) \, u_n(r') \, M(k_n, t), \qquad (r, r') < R. \tag{2.31}$$

Having obtained our basic result, we proceed to the determination of $\psi(r, t)$ for an arbitrary initial condition $\psi(r, 0)$.

C. *Expansion of* $\psi(r, t)$

If our initial state is $\psi(r, 0)$ instead of $\delta(r - r')$, it is clear that at time t $\psi(r, t)$ is given by the integral

$$\psi(r, t) = \int_0^R \psi(r', 0) \, g(r, r', t) \, dr'. \tag{2.32}$$

We define now C_n and $\bar{C}_n$ by the expressions

$$C_n \equiv \int_0^R \psi(r, 0)\, u_n(r)\, dr; \qquad \bar{C}_n = \int_0^R \psi^*(r, 0)\, u_n(r)\, dr, \tag{2.33}$$

where, respectively, $u_n(r)$ is normalized according to Eq. (2.19) and $\psi(r, 0)$ as

$$\int_0^R |\psi(r, 0)|^2\, dr = 1. \tag{2.34}$$

Finally, we can write $\psi(r, t)$ as

$$\psi(r, t) = \sum_{n=-\infty}^{\infty} C_n u_n(r)\, M(k_n, t); \qquad (r < R). \tag{2.35}$$

The coefficients (2.33) obey some useful relations. Multiply both Eqs. (2.23) and (2.24), respectively, by $\psi(r, 0)$ and $\psi^*(r', 0)$ and integrate the result from the origin up to the radius R to obtain [6],

$$\sum_{n=-\infty}^{\infty} \frac{C_n \bar{C}_n}{k_n} = 0 \tag{2.36}$$

and

$$\tfrac{1}{2} \sum_{n=-\infty}^{\infty} C_n \bar{C}_n = 1. \tag{2.37}$$

D. *Expansion of the Survival and Nonescape Probabilities*

From (2.1), (2.33), and (2.35) we get that

$$A(t) = \sum_{n=-\infty}^{\infty} C_n \bar{C}_n M(k_n, t), \tag{2.38}$$

It is worth mentioning that as long ago as 1951, Moshinsky had given an exact expression of $A(t)$ for the one-level case, i.e., when only $k_{\pm 1} \neq 1$, see Eq. (27b) of Ref. [29]. Substitution of Eq. (2.38) into Eq. (2.2) leads to the expression for the survival probability,

$$S(t) = \sum_{n=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} C_n \bar{C}_n C_l^* \bar{C}_l^* M(k_n, t)\, M^*(k_l, t). \tag{2.39}$$

Using $\psi(r, t)$, as given by (2.35), one may obtain an expression for the nonescape probability $P(t)$ with the help of (2.3). We only need to add the definition

$$I_{nl} = \int_0^R u_l^*(r)\, u_n(r)\, dr \tag{2.40}$$

to obtain

$$P(t) = \sum_{n=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} C_n\, C_l^*\, I_{nl}\, M(k_n, t)\, M^*(k_l, t). \tag{2.41}$$

Thus, we have the general expressions for the probabilities of survival and non-escape in the form of a double sum involving the products $M(k_n, t)\, M^*(k_l, t)$ of functions defined by (2.29), with coefficients of the type C_n, $\bar{C}_n$, I_{nl} given respectively by (2.33) and (2.40). Notice that the only difference between both expansions is that in $P(t)$, I_{nl} replaces the product $\bar{C}_n^* \bar{C}_l^*$ that appears in $S(t)$.

E. Exponential and Long Time Behaviour

Equations (2.38), (2.39), and (2.41) are given in terms of M functions and therefore their exponential behaviour is not exhibited explicitly. This can be achieved by using the symmetry relations between the poles on the third and fourth quadrants, $k_{-p} = -k_p^*$, to write the sums only over the poles k_p located on the fourth quadrant and make use of the relation [6, 28],

$$M(k_p, t) = e^{-ik_p^2 t} - M(-k_p, t), \tag{2.42}$$

where $M(-k_p, t)$ is defined as in Eq. (2.29) but with the argument $u = \exp(-i\pi/4)\, k_n t^{1/2}$, instead of (2.30). Using the above relation, the survival amplitude (2.38) may be written as

$$A(t) = \sum_{p=1}^{\infty} C_p\, \bar{C}_p\, e^{-ik_p^2 t} - I(t) \tag{2.43}$$

that displays explicitly the exponentially decaying behaviour, recalling that $k_p^2 = \varepsilon_p - i\Gamma_p/2$. The term $I(t)$ on the right-hand side of the above equation stands for the nonexponential contribution and it reads

$$I(t) = \sum_{p=1}^{\infty} [\, C_p\, \bar{C}_p\, M(-k_p, t)] - C_p^*\, \bar{C}_p^*\, M(-k_p^*, t)], \tag{2.44}$$

where we have used that $C_{-p}\, \bar{C}_{-p} = C_p^*\, \bar{C}_p^*$ and $k_{-p} = -k_p^*$. The argument of the function $M(-k_p^*, t)$ is $u = \exp(-i\pi/4)\, k_p^* t^{1/2}$. Notice that the sums in Eqs. (2.43) and (2.44) run over the same set of poles. The nonexponential contribution given by Eq. (2.44) appears as an infinite sum of terms on the same footing that the description of the exponentially decaying terms. It is worth mentioning that

Khalfin was the first author to discuss nonexponential contributions to decay in general. He used models involving a single resonance term [32]. In other treatments, the nonexponential contribution appears as a complicated integral term and, in general, has been treated in an approximate way [2, 26, 27, 33].

If one ignores the nonexponential contribution $I(t)$ in Eq. (2.43) and furthermore assumes that the initial state is very close to the sharpest resonant state, say the sth, then from (2.36) and (2.37) it follows that $C_s \bar{C}_s \approx 1$, all other coefficients being very small, then (2.43) may be written as $A(t) = e^{-ik_s^2 t}$ and the survival probability becomes the well-known expression

$$S(t) = e^{-\Gamma_s t}. \tag{2.45}$$

A similar analysis can be done for the nonescape probability. Noticing that $I_{ss} \approx 1$, as follows from inspection of (2.19) and (2.40), one obtains

$$P(t) = e^{-\Gamma_s t}. \tag{2.46}$$

The equivalence of $S(t)$ and $P(t)$ as shown above, along the exponentially decaying region, has probably led to confusion regarding the notions of survival and nonescape probabilities.

Let us now turn to the analysis of the long time behavior. From Eq. (2.42) 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^*. Indeed from the definition of the function M, given by (2.29), one may get the asymptotic expansion of $\exp(u^2)\,\mathrm{erfc}(u)$ to obtain [6, 28]

$$M(-k_n, t) \approx \frac{i}{2(\pi i)^{1/2}} \left(\frac{1}{k_n t^{1/2}} \right) - \frac{1}{4(\pi i)^{1/2}} \left(\frac{1}{k_n^3 t^{3/2}} \right) + \cdots. \tag{2.47}$$

Substitution of Eq. (2.47) into (2.44) allows us to write $I(t)$ as a sum over terms that go like inverse powers of time. One may see, however, that the coefficient proportional to $t^{-1/2}$, is identical to Eq. (2.36) and therefore it cancels out exactly. Consequently the survival amplitude (2.43) may be written as

$$A(t) \approx \sum_{p=1}^{\infty} \left[C_p \bar{C}_p e^{-ik_p^2 t} - \frac{1}{4(\pi i)^{1/2}} \left[\frac{C_p \bar{C}_p}{k_p^3} - \left(\frac{C_p \bar{C}_p}{k_p^3} \right)^* \right] \frac{1}{t^{3/2}} + \cdots \right]. \tag{2.48}$$

The above equation exhibits the crossover from exponential to a power law behaviour. Using (2.48) one sees that the survival probability (2.39) behaves at long times as $S(t) \sim t^{-3}$.

Let us now consider the long time behaviour of the nonescape probability. One sees from Eq. (2.31) into Eq. (2.3) 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 originated the integrals I_{nl} defined by (2.40). Hence, when the asymptotic expansion of the M

functions (2.47) is introduced into (2.41), the leading contribution is proportional to t^{-1} and includes terms of the type

$$\sum_{r}^{\infty} \sum_{r}^{\infty} \left(\frac{C_r^* C_s I_{rs}}{k_r^* k_s} \right) \frac{1}{t}, \tag{2.49}$$

that are different from (2.36) and, hence, do not cancel. In other words, asymptotically, $P(t) \sim t^{-1}$. One concludes, therefore, that the survival and the nonescape probabilities behave with a different inverse power of time for long times [1].

The previous discussion refers only to resonant states; however, it can be easily extended to include bound states [6]. In such a case the long time behaviour of the survival and nonescape probabilities has a nonvanishing asymptotic value due to the oscillating character of the time dependence of the bound states. For instance, if in addition to resonant states there is a bound state, as time goes to infinity the survival probability reads

$$S(t) = |C_b|^2, \tag{2.50}$$

where C_b and $\bar{C}_b = C_b^*$ stand for the overlap integrals defined in Eq. (2.33) with the $u_n(r)$ replaced by the bound state function $u_b(r)$. The above nonvanishing asymptotic value for the survival probability is sometimes referred to in the literature as population trapping [8]. Proceeding in a similar fashion as above for the nonescape probability yields, in the limit that the time goes to infinity, that

$$P(t) = |C_b|^2. \tag{2.51}$$

One sees that both $S(t)$ and $P(t)$ provide at very long times a similar result when bound states enter into the problem.

III. EXAMPLE

We shall now consider a problem that illustrates numerically the behaviour of $S(t)$ and $P(t)$. We take $V(r)$ as a delta-function potential

$$V(r) = b\delta(r - 1), \tag{3.1}$$

with strength b and where we choose $R = 1$. For the initial condition we take

$$\psi(r, 0) = \begin{cases} \beta(\kappa) \sin \kappa r, & \text{if } 0 \leqslant r \leqslant 1, \\ 0, & \text{if } r > 1, \end{cases} \tag{3.2}$$

where κ is an arbitrary real parameter and, for normalization, we require that

$$\beta(\kappa) = \sqrt{2}[1 - (2\kappa)^{-1} \sin 2\kappa]^{-1}. \tag{3.3}$$

The form (3.2) was suggested by the fact that if $b \to \infty$, the normalized stationary states for the problem are

$$\psi(r, 0) = \begin{cases} \sqrt{2} \sin m\pi r, & \text{if} \quad 0 \leqslant r \leqslant 1; \ m = 1, 2, 3, ..., \\ 0, & \text{if} \quad r > 1, \end{cases} \tag{3.4}$$

and so an interesting question could be what happens at any time t if at $t = 0$ we consider the above initial state. This state implies that initially we are very close to a resonance, and since we would like to consider also the case of an initial state situated between two resonances, we use the more general form (3.2).

From (2.15) we immediately see that

$$u_n(r) = d_n \sin k_n r, \tag{3.5}$$

where d_n and the equation satisfied by k_n will be given below. Using (3.5) we see that Eq. (2.17) has to be modified to take into account the fact that the delta-function potential is discontinuous at $r = R = 1$. Hence for this example instead of Eq. (2.17) we have the condition

$$ik_n u_n(1) - \left[\frac{du_n(r)}{dr} \right]_{r = R_- = 1_-} = bu_n(1). \tag{3.6}$$

Substitution of Eq. (3.5) into the above expression yields the equation for the complex eigenvalues of the problem, namely,

$$2ik_n + b(e^{2ik_n} - 1) = 0. \tag{3.7}$$

The solutions to the above trascendental equation correspond also to the poles k_n ($n = \pm 1, \pm 2, \pm 3, ...$), of $G^+(r, r'; k)$ and in this case all of them are in the lower half of the k plane with $k_{-n} = -k_n^*$.

The coefficient d_n in Eq. (3.5) may be obtained from the normalization condition given by Eq. (2.19). Using (3.7) it may be written as

$$d_n = \left[\frac{2(b - 2ik_n)}{(1 + b - 2ik_n)} \right]^{1/2}. \tag{3.8}$$

In order to calculate the survival and nonescape probabilities, given respectively by (2.39) and (2.41), we need to determine also the coefficients C_n and I_{nl} using (3.5) for $u_n(r)$ and (3.2) for $\psi(r, 0)$. Since the initial condition $\psi(r, 0) = \beta(\kappa)\sin \kappa r$ depends on the parameter κ, we shall denote C_n as $C_n(\kappa)$. Hence from (2.33) we obtain

$$C_n(\kappa) = \beta(\kappa) \, d_n \, \frac{k_n e^{-ik_n}}{b(\kappa^2 - k_n^2)} \left[\kappa \cos \kappa - i(k_n + ib) \sin \kappa \right]. \tag{3.9}$$

Note that as our initial state (3.5) is real $C_n = \bar{C}_n$. On the other hand, from (2.40) and (3.5)

$$I_{nl} = i \frac{d_n d_l^* k_n k_l^*}{b^2(k_l^* - k_n)} e^{i(k_l^* - k_n)}, \tag{3.10}$$

where for all of these coefficients we have made use of the fact that, from (3.7), k_n satisfies

$$e^{2ik_n} = \frac{2k_n + ib}{ib}. \tag{3.11}$$

Substitution of the coefficients given by (3.8), (3.9), and (3.10) in (2.39) and (2.41), leads to explicit analytic expressions for the probabilities of survival $S(t)$ and nonescape $P(t)$ that we now proceed to discuss.

An interesting case refers to sharp isolated resonances. For not very highly excited resonances, this case can be achieved by taking a large value for the intensity of the potential, namely, in our units, $b \gg 1$. In that case, as shown in Ref. [28], the poles of $G^+(r, r'; k)$ are given approximately by

$$k_n \simeq n\pi \left(1 - \frac{1}{b}\right) - i \left(\frac{n\pi}{b}\right)^2. \tag{3.12}$$

A. *Comparison of $S(t)$ and $P(t)$*

We shall analyze the survival and nonescape probabilities when $b \gg 1$ and $\kappa = m\pi$. The complex energy E_n associated with k_n of (3.12) is approximately given by

$$E_n = k_n^2 \simeq n^2\pi^2 - 2i \frac{n^3\pi^3}{b^2}, \tag{3.13}$$

so that the separation of the resonances, i.e., the real part of the difference $E_{n+1} - E_n$, is much larger than the width of one of them, i.e., the imaginary part of E_n. The choice $\kappa = m\pi$ implies that the initial state (3.2) is associated with an energy $\kappa^2 = m^2\pi^2$ and this it is very close in energy to the corresponding resonance as follows from (3.13) with $n = m$. Since $\beta(m\pi) = (2)^{1/2}$, we see that the formula (3.9) for $C_n(m\pi)$ becomes

$$C_n(m\pi) \approx \frac{2nm}{b(m^2 - n^2)}; \qquad n \neq m, \tag{3.14}$$

that has a large factor b in the denominator. On the other hand for $n = m$, we have from (3.12), that $(m^2\pi^2 - k_m^2) \approx (2m^2\pi^2/b)$ and thus

$$C_m(m\pi) \approx 1. \tag{3.15}$$

We can also analyze for $b \gg 1$, and b much larger than n and l, the behaviour of I_{nl}. We get from (3.10) and (3.11) that

$$I_{nl} \approx \frac{2inl\pi}{b^2(l-n)}; \qquad n \neq l, \tag{3.16}$$

and

$$I_{nn} \approx 1. \tag{3.17}$$

Thus, if $b \gg 1$, and also b much larger than m, and the initial state is very close to the mth resonant state, we see from (3.14), (3.15), and (3.17) that the survival and nonescape probabilities essentially reduce to

$$S(t) \approx P(t) \approx e^{-\Gamma_m t} = e^{-t/\tau}, \tag{3.18}$$

with τ defined as

$$\tau = \frac{b^2}{4m^3\pi^3}. \tag{3.19}$$

Hence, when we are close to a narrow resonance, the survival and nonescape probabilities coincide for a number of lifetimes until the contribution of the resonance with the largest lifetime dominates the time evolution of $S(t)$ and $P(t)$, as will be shown in the numerical examples presented in the next section.

On the other hand, when the initial state is between resonances, i.e., $\kappa = (m+1/2)\pi$, inspection of Eq. (3.9) yields

$$C_n((m+1/2)\pi) \approx -\frac{2in}{(m^2-n^2)\pi}; \qquad n \neq m, \tag{3.20}$$

and for $n = m$,

$$C_n((n+1/2)\pi) \approx -\frac{2i}{\pi}, \tag{3.21}$$

which indicates that there is no a single coefficient C_n that dominates over the expansions for $S(t)$ or $P(t)$. Hence, there is no reason to expect initially an exponential decay law behaviour. In the next section we also exemplify this situation.

B. Numerical Results

In order to analyze $S(t)$ and $P(t)$ we need to specify two parameters: the strength b of the delta-function potential and the wavenumber k for the initial condition. In what follows, we will take the fixed value $b = 100$. On the other hand, we have to find the poles k_n in the complex k-plane that satisfy Eq. (3.7). In order to do so, we use the well-known Newton–Raphson method to locate the poles in the fourth

quadrant k_n ($n = 1, 2, ..., N$); the remaining poles lie on the third quadrant and are given by $k_{-n} = -k_n^*$. We have considered in our calculations 1000 poles ($N = 500$); those on the fourth quadrant are depicted in Fig. 4. Notice that the real part of k_n is much larger than the imaginary part of k_n and, as a consequence, we are in a regime in which the real part of the complex energy E_n is much larger than its imaginary part; that is, we are dealing with sharp isolated resonances. The poles in Fig. 4 depend on the parameter b, and when $b \gg 1$ they are given approximately by Eq. (3.12). In fact, we use (3.12) as an input for the Newton–Raphson algorithm, in order to obtain the exact location of the poles. When $b \to \infty$, the poles "move" to the real axis in the k-plane and are given by $k_n = n\pi$; this limiting case corresponds to the bound states of a particle in a box.

Once we have obtained the analytical expression for the survival $S(t)$ and non-escape $P(t)$ probabilities (Eqs. (2.39) and (2.41)), we can analyze both quantities numerically. As mentioned above we will take $b = 100$. In the remaining figures we plot the logarithm of $S(t)$ as a solid line and the logarithm of $P(t)$ as a dashed line. In Fig. 5 we show $\ln S(t)$ and $\ln P(t)$ as a function of time, when the initial condition has a value $\kappa = 5\pi$. This value corresponds to an initial state close to the fifth resonance and hence refers to the time evolution of an initial state at a higher excitation energy to those considered in Ref. [1] where the initial states were considered, respectively, near the first and second resonances of the system. The fifth resonance has a lifetime $\tau_5 = 1/\Gamma_5$, where Γ_5 is its width. We will take the time in Figs. 5 and 6 in units of τ_5.
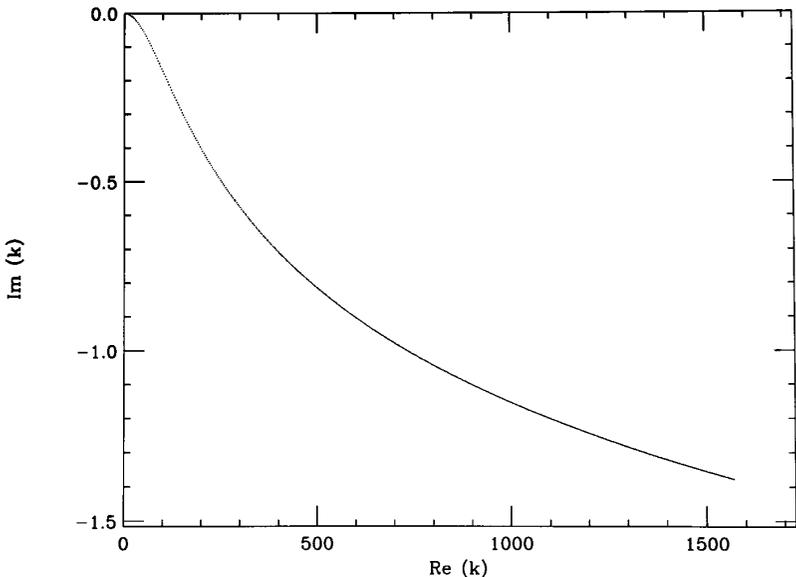

FIG. 4. Location of the first 500 poles k_n, given by Eq. (3.7), in the complex k-plane. Only the fourth quadrant is shown and notice that $\text{Re}(k) \gg \text{Im}(k)$.
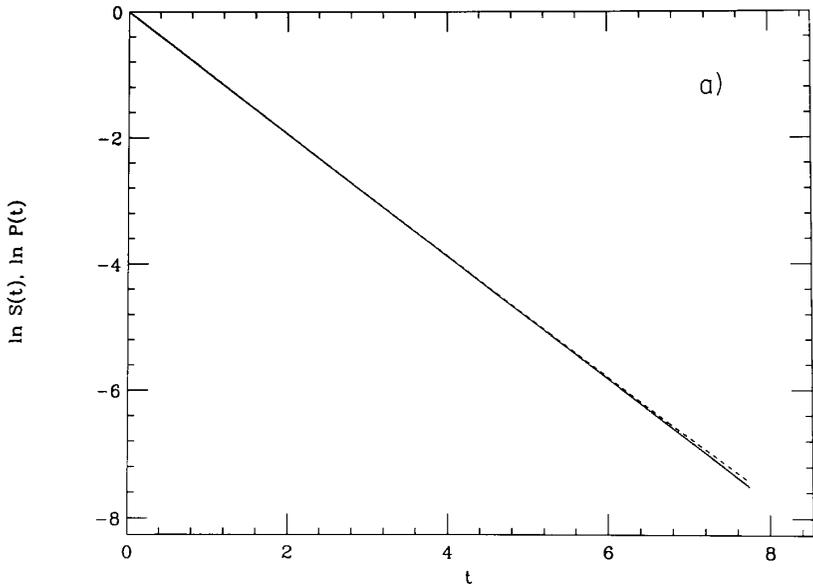
FIG. 5.   Logarithm of the survival (solid line) and nonescape (dashed line) probabilities as a function of time, for $b = 100$ and the resonance case $k = 5\pi$. The time scale is given in units of τ_5. (a) At the beginning of the decay process both quantities coincide and decay exponentially with a lifetime τ_5. The slope is given by $\Gamma_5 = 1/\tau_5$. (b) After a time $\simeq 10\tau_5$, $S(t)$ and $P(t)$ separate from each other, and both probabilities start to decay with a lifetime τ_1, which corresponds to the ground state. Notice the oscillations for $S(t)$ during the crossover from the excited state (slope Γ_5) to the ground state (slope Γ_1). (c) For very long times ($6000 \, \tau_5$) we can clearly see three separate regions for both $S(t)$ and $P(t)$: the exponential region with slope Γ_5 at the beginning; the crossover to the ground state with slope Γ_1; and finally, another crossover to a power law decay, in which $S(t) \sim t^{-3}$ and $P(t) \sim t^{-1}$.

We see from Fig. 5a that at the beginning of the decay process, both quantities coincide and both decay exponentially with a lifetime τ_5, as expected from the choice of the initial condition. As is well known [28] the exponential decay is not valid for very small times, i.e., times much smaller than a lifetime, however this deviation cannot be appreciated in our figures due to the scale. In Fig. 5b we can see that after a time $\approx 10\tau_5$, $S(t)$ and $P(t)$ separate from each other; $S(t)$ decays exponentially with a slope Γ_5 for about 20 lifetimes ($t \approx 20\tau_5$). After that time, something interesting happens: $S(t)$ starts to oscillate and then decay exponentially once again, but this time with a lifetime τ_1 which corresponds to the ground state of the system. The nonescape probability $P(t)$, after a time $\approx 10\tau_5$, change the slope of the exponential decay from Γ_5 to Γ_1, but in a smooth way without any oscillations. Finally, in Fig. 5c, we show the behavior of $S(t)$ and $P(t)$ from the beginning of the decay process until very long times ($t/\tau_5 = 6000$) in order to analyze the asymptotic decay. We can clearly see three separate regions for both $S(t)$ and $P(t)$: the exponential region with slope Γ_5 at the beginning; the crossover to an exponential decay with slope Γ_1 corresponding to the ground state and; another
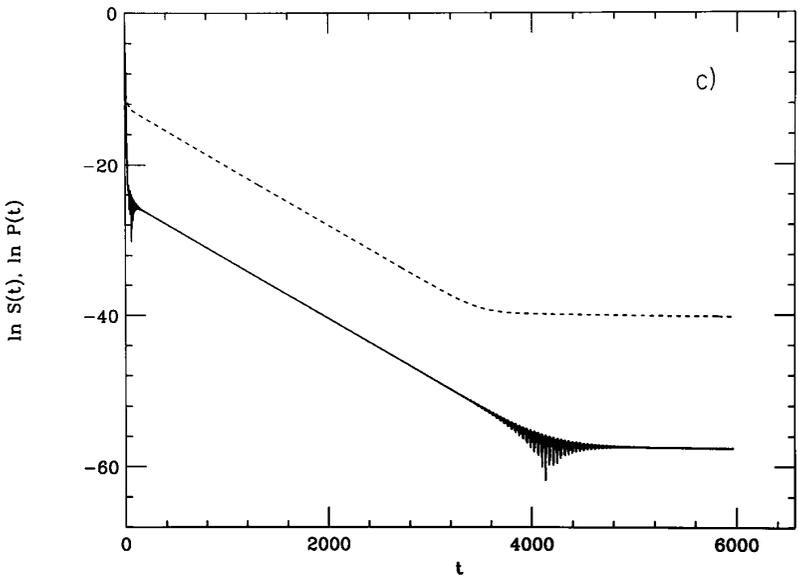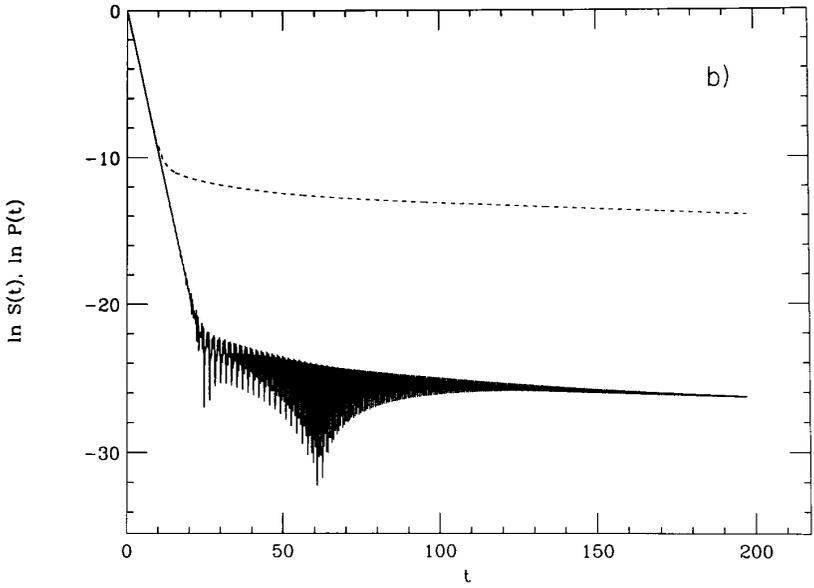
FIG. 5.—*Continued*

crossover (for $\tau/\tau_5 \approx 4000$) to a power law decay in which $S(t) \sim t^{-3}$ and $P(t) \sim t^{-1}$. Notice that $P(t)$ is always a smooth function and that $S(t)$, on the other hand, fluctuates during the transitions from one regime to another.

Before we analyze the nonresonant case, let us try to understand the results depicted in Fig. 5. First of all, when we choose an initial condition $\psi(r, 0)$ such that $k = m\pi$, with m an integer, we are very close to a resonance given by the pole k_m. In this case we have a leading term for $S(t)$ and $P(t)$ due to the resonant denominator of the form $(m^2\pi^2 - k_m^2)^{-1}$. The presence of this leading term guarantees an exponential decay with a lifetime $\tau_m = \Gamma_m^{-1}$, associated with the complex energy $E_m = \varepsilon_m - i\Gamma_m/2$. Furthermore, as discussed above, when $k = m\pi$ and $b \gg 1$, $P(t)$ and $S(t)$ coincide. This is precisely what we found in the example shown in Fig. 5a, when $m = 5$.

Now, in order to understand the crossover to the ground state with a lifetime $\tau_1 = \Gamma_1^{-1}$, we have to remember that in our example there exist an ordering $\tau_1 > \tau_2 > \cdots > \tau_N$; that is, the ground state is the state with the longest lifetime and therefore it dominates the decay process at long times. In terms of the widths, the first resonance is the thinnest. The fluctuations obtained for $S(t)$ in the interval $20\tau_5$ to $200\tau_5$ in Fig. 5b, correspond to the interplay of all the states between $m = 1$ and $m = 5$. In addition to the cases $m = 1$ and $m = 2$ considered in Ref. [1], we have also analyzed the case in which $m = 3$ (not shown here), where $S(t)$ decays exponentially with a lifetime τ_3 at the beginning and, during the crossover to the ground state, it oscillates periodically with a period given by $(\varepsilon_2 - \varepsilon_1)^{-1}$.

Finally, as discussed for the general case of a finite range potential (Section II), the asymptotic behaviors of $S(t)$ and $P(t)$ are governed by the asymptotic form of the function $M(k_n, t)$ and the sum rules given by (2.36) and (2.37). The result is that we obtain numerically for the delta-function potential that $S(t) \sim t^{-3}$ and $P(t) \sim t^{-1}$, as expected.

Let us now turn to the nonresonant case in which κ is not a multiple of π. We choose $\kappa = 5.5\pi$, which corresponds to an initial state situated between two resonances, i.e., $m = 5$ and $m = 6$. In Fig. 6 we show $\ln S(t)$ and $\ln P(t)$ as a function of time, in units of τ_5. Once again, the dashed line correspond to $\ln P(t)$ and the solid line to $\ln S(t)$. In Fig. 6a we can see that at the beginning of the decay process neither $S(t)$ nor $P(t)$ decay exponentially. $P(t)$ is a smooth curve but $S(t)$ fluctuates much more strongly than the resonant case during the entire process. For longer times ($t/\tau_5 \approx 100$), both quantities start to decay exponentially with a lifetime τ_1, as can be seen in Fig. 6b, even though we are in the off-resonance case characterized by $\kappa = 5.5\pi$. Finally, in Fig. 6c we can see a crossover, for very long times ($t/\tau_5 \approx 3000$), to a power law decay. Once again, in this regime $S(t) \sim t^{-3}$ and $P(t) \sim t^{-1}$.

Let us try to understand the differences between $P(t)$ and $S(t)$ from a physical standpoint. The nonescape probability $P(t)$ is, by definition, the probability that a particle remains confined inside a certain region. Thus, the particle can change from the initial state to another state inside the potential and this change does not affect $P(t)$. The only way in which $P(t)$ can decrease is when the particle leaves the
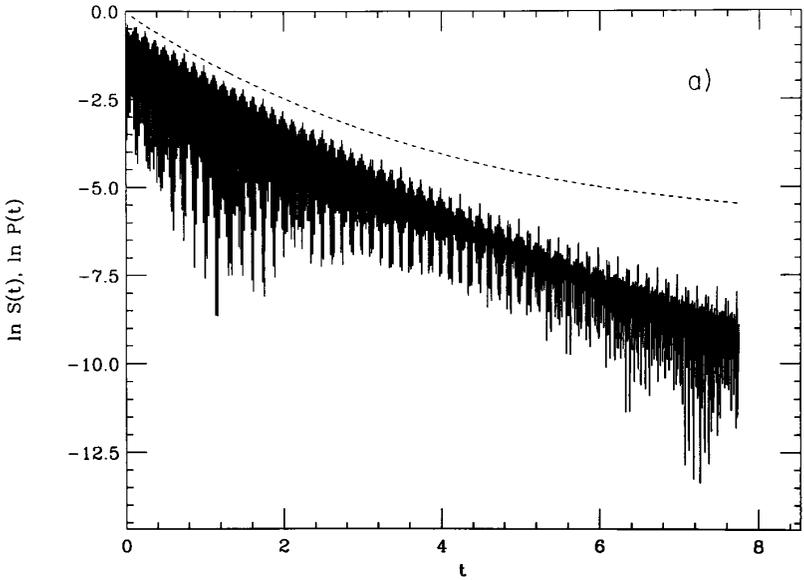
FIG. 6. Logarithm of the survival (solid line) and non-escape (dashed line) probabilities as a function of time, for $b = 100$ and the nonresonance case $k = 5.5\pi$. The time scale is given in units of τ_5. (a) In contrast to the resonance case (see Fig. 5a), neither $S(t)$ nor $P(t)$ decay exponentially, and $S(t)$ displays a fluctuating character. (b) Although we are in the off-resonance case, after some time, $S(t)$ and $P(t)$ start to decay with a lifetime τ_1, which corresponds to the ground state. (c) For very long times ($\approx 4000\tau_5$) we can distinguish three separate regions for $S(t)$ and $P(t)$: a non exponential region at the begining; the crossover for the ground state with slope Γ_1; and finally, the transition to a power law decay, in which $S(t) \sim t^{-3}$ and $P(t) \sim t^{-1}$.

potential region, say by tunneling. In the problem we are analyzing, once outside, the particle cannot enter this region again and, therefore, we expect a decreasing smooth curve describing the nonescape probability. On the other hand, the survival probability $S(t)$ refers to the probability that a particle remains after a time t in its initial state, where the latter is confined inside the potential region. Suppose that a particle is initially between two resonances. Before the particle leaves the potential region, it can make transitions from one state to another and return to the initial state and so on. All these transitions are manifested by the rapid oscillations of the survival probability.

A result of our analysis that seems of interest to stress here is that, independently on the conditions for the initial state, eventually the resonant state with the longest lifetime predominates over the time evolution of decay. Apparently the system loses memory on whether the initial state is close to the mth or the nth resonance, or between the mth and the nth resonances. The last stage of the decaying process proceeds always exponentially before the croosover to the power law decay takes over. Indeed, at the beginning of the decay proccess the differences in the time evolution for different initial states may be dramatic, as shown, for example, by
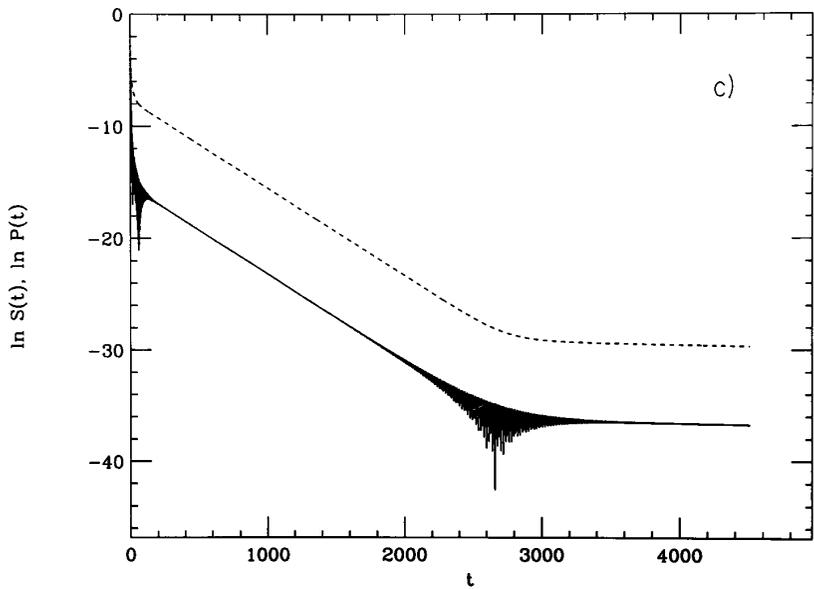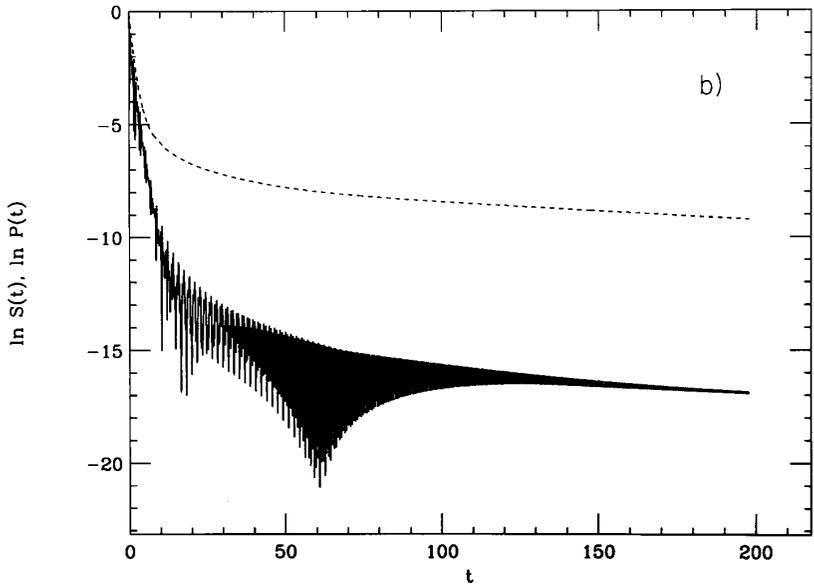
FIG. 6.—*Continued*

Figs. 5a and 6a, and also by Figs. 5b and 6b. However, once the transition to the first resonance occurs the decay out of this state and the crossover to the power law behaviour becomes similar to that shown by Figs. 5c and 6c.

The above situation may be understood in general by inspection of Eq. (2.37) in view of (2.39) and (2.41) for $S(t)$ and $P(t)$, respectively, and using the relation (2.42) to exhibit the exponential dependence of the above definitions explicitly. The initial state determines the values of the different coefficients $C_n \bar{C}_n$ and the main point is to realize that for the longest lived state, say the sth, even if the coefficient $C_s \bar{C}_s$ is small, the product $C_s \bar{C}_s \exp(-ik_s^2 t)$ will eventually dominate over all other exponentially decaying terms. This follows because the other decaying terms, having smaller lifetimes, go to zero much faster.

IV. CONCLUDING REMARKS

In this work we have made use of an exact expansion for the retarded time dependent Green function in terms of resonant states to study the time evolution of an initially confined arbitrary state. Our approach allows us to treat both the exponential and nonexponential contributions to the time evolution of decay on the same footing. We have compared the notions of the survival and nonescape probabilities and found that, in general, they exhibit a different behaviour with time. For the case of an initial state close to a resonance the above notions coincide along the exponentially decaying region. However, if the initial state is not close to a resonance these probabilities exhibit a nonexponential behaviour. In the above two cases, we have shown that eventually the resonance with the longest lifetime predominates in the decay process which may be seen as a "loss of memory" of the initial condition. This occurs in an exponential fashion before the onset to a power law decay is established, i.e. $S(t) \sim t^{-3}$ and $P(t) \sim t^{-1}$. However in the case that bound states are present both quantities tend to a constant, i.e., $S(t) \sim P(t) \sim |C_b|^2$.

The above formulation may be generalized to bidimensional systems, in particular to systems with arbitrary geometries [3]. Also, our formulation may be of interest in studies of the tunneling dynamics of squeezed states [12] and in the time evolution of chaotic quantum systems, where nonexponential decay have also been obtained [35–37]. Here it could be of interest, for example, to investigate the role of the power law decay for the case of quantum systems that behave chaotically in the classical limit. Furthermore, our results might be of interest in the efforts to verify experimentally the nonexponential contributions to decay [7]. For nuclear radioactive decay it has been reported [9] no deviation from exponential decay up to 45 half-lives for the case of Mn^{56}. A more promising possibility to observe nonexponential contributions to decay could be in photodetachment near the threshold in atomic physics [8, 38, 39]. The analysis of the present work could be of interest in that field because negative ions in photodetachment near the threshold are usually modelled by a single electron in a short-range potential.

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