Analytical approach to the wave function of a decaying quantum system

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(Received 1 September 2001; published 16 January 2002)

Recently we outlined an analytical method of solving the time-dependent Schrödinger equation for a model which simulates a decaying quantum system such as an α-decaying nucleus. A particle in the model is initially confined around the origin and leaks out, tunneling through a potential barrier. The solution can be expressed as a linear combination of the Moshinsky functions, each of which is associated with a pole of the scattering **S** matrix of the model. In this paper we give a full account of the method with a few explicit examples. We examine deviations from the exponential decay law at very large times. We comment on a recent controversy regarding the t dependence of the survival and nonescape probabilities when t is very large.

DOI: 10.1103/PhysRevC.65.024608 PACS number(s): 03.65.−w, 12.39.Ba, 12.39.Ki

I. INTRODUCTION

We consider a model which simulates a decaying quantum system such as an α-decaying nucleus [1–5]. The model assumes that a particle is initially confined within a region around the origin and at a certain time, $t=0$, it begins to leak out by tunneling through a potential barrier. This problem is intrinsically time dependent. Let us confine ourselves to the S state. We assume that the solutions of the Schrödinger equation for the stationary states of the model are all known. Then the wave function $\psi(r,t)$ of any nonstationary state can be expressed as a linear superposition of stationary wave functions. For a given initial wave function $\psi(r,0)$, the coefficients of the superposition can be determined. In this sense any time-dependent problem including that of the decay process is solvable. It is, however, highly nontrivial to calculate $\psi(r,t)$ of this form of superposition explicitly, in particular, for large values of r and/or t. Alternatively one can solve the time-dependent Schrödinger equation numerically [6–10]. This, however, becomes again prohibitive as r and/or t become very large.

Recently [11,12] we outlined a new method which enables us to obtain the $\psi(r,t)$ of the decay problem as a linear combination of Moshinsky functions [13–15], each of which is associated with a pole of the scattering **S** matrix of the model. In this way we can calculate the wave function accurately regardless of the magnitude of r and t. The applicability of the method is limited to models for which the stationary solutions of the Schrödinger equation are known analytically. Such models still exhibit rich physics of the decay process. The method is powerful in analyzing the behavior of $\psi(r,t)$ of the models for very large values of r and t. There are significant problems that require knowledge of $\psi(r,t)$ for very large values of r and t; for example, the atomic ionization caused by the nuclear α decay [16], and bremsstrahlung in α decay [8,9]. There is a similar problem regarding β decay [10].

The purpose of this paper is to give a full description of the new method with a few illustrations. The method facilitates exploring various features of the decay process. In the light of the exact wave function, we reexamine the so-called Gamow wave function that has been used extensively in the literature [17–25]. As is well known the Gamow wave function is not normalizable in the usual way. This is related to the fact that the Gamow wave function consists of only an outgoing wave at and outside the potential barrier. On the other hand the exact wave function always contains, in addition to outgoing waves, an admixture (although usually small) of incoming waves. This implies that the exact wave function cannot simply be expressed as a superposition of Gamow-type wave functions. We also examine the t dependence of the survival and nonescape probabilities when t becomes very large. Contrary to what was reported in Refs. [22–24], we find that these probabilities (in the absence of stationary bound states) both behave like t^{-3} as t becomes very large. The wave function used in Refs. [22,24,25], being a superposition of Gamow-type wave functions, is not exact.

In Sec. II we explain the basic idea that underlies the method and develop the theory. In Sec. III we examine examples of the method with a δ-function potential, a square-barrier potential, and their generalizations. In Sec. IV we discuss the Gamow wave function. In Sec. V we examine the t dependence of the survival and nonescape probabilities when t is very large. A summary is given in Sec. VI. In Appendix A we give some details of the Moshinsky function. In Appendix B we expand on the numerical evaluation of the poles of the **S** matrix and the summation to obtain the wave functions. In Appendix C we consider a potential that is a combination of many square barriers or wells. This is an extension of the examples of Sec. III.

II. MODEL AND BASIC STRATEGY

We assume a central potential $V(r)$ such that it has a repulsive barrier which supports one or more unstable bound states or resonances. There may or may not be stable bound states. Furthermore we assume that

$$V(r)=0 \qquad \text{for} \qquad r>a. \tag{1}$$

It is also understood that $\int_0^\infty rV(r)dr$ is finite. (These assumptions are not literally valid for α decay because of the

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Coulomb potential.) We use units such that $\hbar=1$ and $2m=1$ throughout. We confine ourselves to the S state and attempt to obtain the solution $\psi(r,t)$ (actually the wave function times r) of the time-dependent Schrödinger equation for $t>0$,

$$i\frac{\partial\psi(r,t)}{\partial t}=\left[-\frac{\partial^2}{\partial r^2}+V(r)\right]\psi(r,t),\quad \psi(0,t)=0. \tag{2}$$

It is understood that the wave function starts with a given normalized $\psi(r,0)$ that represents the state in which the particle is initially confined to $r<a$.

We assume that the stationary solutions of the Schrödinger equation are all known. Let us write the scattering solutions as

$$\psi(k,r,t)=e^{-ik^2t}u(k,r), \tag{3}$$

$$u(k,r)=\frac{1}{2ik}[f(k)f(-k,r)-f(-k)f(k,r)], \tag{4}$$

where $k>0$ and k^2 is the associated energy [26]. The $f(k,r)$ is the Jost solution of the time-independent Schrödinger equation with energy k^2. It is normalized such that $e^{ikr}f(k,r)=1$ when $r>a$. The $f(k)$ is the Jost function that is related to $f(k,r)$ by $f(k)=f(k,0)$. The Jost solution is complex but $f^*(k,r)=f(-k,r)$ and hence $u(k,r)$ is real. Furthermore $u(k,r)$ is an even function of k. The $u(k,r)$ is normalized such that

$$\int_0^\infty u(k,r)u(k',r)dr=\frac{\pi}{2k^2}|f(k)|^2\delta(k-k'). \tag{5}$$

The $f(k)$ is related to the scattering phase shift $\eta(k)$ and the **S** matrix by

$$f(k)=|f(k)|e^{i\eta(k)},\qquad \mathbf{S}(k)=\frac{f(k)}{f(-k)}. \tag{6}$$

In the above we assumed that k is a real variable. In the following, however, it is understood that k can be complex. If $f(-k)=0$ for $k=i\kappa(\kappa>0)$, the **S** matrix obtains a pole at $k=i\kappa$. This leads to a stable bound state of energy $-\kappa^2$. Let its normalized wave function be

$$\psi_\kappa(r,t)=e^{i\kappa^2t}u_\kappa(r). \tag{7}$$

For simplicity we assume that there is only one or no bound state. The generalization to cases with more than one bound state is straightforward. The $u(k,r)$ and $u_\kappa(r)$ form a complete orthonormal set. The completeness relation is

$$\frac{2}{\pi}\int_0^\infty\frac{k^2}{|f(k)|^2}u(k,r)u(k,r')dk+u_\kappa(r)u_\kappa(r')=\delta(r-r'). \tag{8}$$

The wave function $\psi(r,t)$ can be expressed in terms of the stationary solutions as

$$\psi(r,t)=\frac{2}{\pi}\int_0^\infty\frac{k^2}{|f(k)|^2}C(k)e^{-ik^2t}u(k,r)dk+C_\kappa e^{i\kappa^2t}u_\kappa(r), \tag{9}$$

where

$$C(k)=\int_0^\infty u(k,r)\psi(r,0)dr, \tag{10}$$

$$C_\kappa=\int_0^\infty u_\kappa(r)\psi(r,0)dr. \tag{11}$$

The $u(k,r)$ is an entire function of complex k and so is $C(k)$. Furthermore, $C(k)\to0$ as $k\to\infty$. This is because $u(k,r)$ tends to its free version $k^{-1}\sin kr$ in this limit while $\psi(r,0)$ is finite. Since $C(-k)=C(k)$ we can write $\psi(r,t)$ as

$$\begin{aligned}\psi(r,t)&=\int_0^\infty e^{-ik^2t}[e^{ik(r-a)}h(k,r)\\&\quad+e^{-ik(r-a)}h(-k,r)]dk+C_\kappa e^{i\kappa^2t}u_\kappa(r)\\&=\int_{-\infty}^\infty e^{-ik^2t}e^{ik(r-a)}h(k,r)dk+C_\kappa e^{i\kappa^2t}u_\kappa(r),\end{aligned} \tag{12}$$

where $h(k,r)$ is defined by

$$h(k,r)=-\frac{i}{\pi}kC(k)\frac{e^{-ik(r-a)}f(-k,r)}{f(-k)}. \tag{13}$$

The function $h(k,r)$ is related to $g(k,r)$ of Ref. [11] by $h(k,r)=g(k,r)e^{ika}$. If $r>a$, then $e^{-ikr}f(-k,r)=1$ and hence $h(k,r)$ is independent of r. The factor $e^{ik(r-a)}$ of the integrand of Eq. (12) cancels $e^{-ik(r-a)}$ of $h(k,r)$. The $h(k,r)$ so defined is free from essential singularities as a function of k when $r>a$. We discuss this point further in Sec. III.

We are assuming that the stationary solutions of the model are all known and hence $h(k,r)$ is known. One may then think that $\psi(r,t)$ can be obtained by simply performing the k integration of Eq. (12). This is true if r is small. For the model of the δ-function potential that we examine in the next section, Winter [5] obtained $\psi(r,t)$ in this manner, but only up to the potential barrier $r=a$. The difficulty in calculating $\psi(r,t)$ for larger values of r in this manner has been discussed in detail in Ref. [6]. In contrast to Eq. (12), Eq. (16) that we derive below enables us to evaluate $\psi(r,t)$ accurately and easily no matter how large r and/or t become.

The $h(k,r)$ as a function of complex k has an infinite number of simple poles, which are due to the zeros of $f(-k)$, which in turn give rise to poles of the **S** matrix. The $h(k,r)$ has no other singularities for finite k. This is so because $f(k,r)$ is an entire function of k when the potential vanishes for $r>a$ [27] as we assumed. In the absence of bound states, these poles are all in the lower-half complex k plane, located symmetrically about the imaginary axis [27]. Let us denote the poles in the fourth quadrant with k_ν,ν

$=1,2,3,\ldots;\mathrm{Re}(k_\nu)$ increases with increasing ν. We also denote the poles in the third quadrant with k_ν, but with $\nu=-1,-2,-3,\ldots$. The poles are symmetrically located; $k_{-\nu}=-k_\nu^*$. If there is a bound state, there is an additional pole on the positive imaginary axis at $k=i\kappa$. Such a bound-state pole may be accompanied by another pole on the negative imaginary axis, which we will denote as $k=i\kappa'$ where $\kappa'<0$. (In all the examples of Sec. III, poles at $i\kappa$ and $i\kappa'$ appear in a pair.) The quantities κ and κ' do not necessarily have the same magnitude. In the following we consider only cases with one or no bound state. In the case of no bound state the terms involving κ or κ' should be dropped from the expressions.

If we assume $r>a$ so that $h(k,r)$ has no essential singularity in k at infinity, the Mittag-Leffler theorem [28] allows us to expand $h(k,r)$ as

$$h(k,r)=\frac{i}{2\pi}\left[\sum_\nu\left(\frac{1}{k-k_\nu}+\frac{1}{k_\nu}\right)c_\nu(r)+\left(\frac{1}{k-i\kappa}+\frac{1}{i\kappa}\right)c_\kappa(r)+\left(\frac{1}{k-i\kappa'}+\frac{1}{i\kappa'}\right)c_{\kappa'}(r)\right], \tag{14}$$

where the summation is over $\nu=\pm1,\pm2,\ldots$. The $c_\nu(r)$, $c_\kappa(r)$, and $c'_\kappa(r)$ are, respectively, the residues associated with the poles of $(2\pi/i)h(k,r)$ at k_ν,κ, and κ'. When $r>a,h(r,k)$ and its residues are all independent of r. Note that $h(0,r)=0$, which is due to the factor k of Eq. (13). Equation (14) is consistent with $h(0,r)=0$. When $r>a$ the residues satisfy

$$\sum_\nu\frac{c_\nu(r)}{k_\nu}+\frac{c_\kappa(r)}{i\kappa}+\frac{c_{\kappa'}(r)}{i\kappa'}=0, \tag{15}$$

since $h(k,r)\to0$ when $k\to\infty$. By using this relation, Eq. (14) can be simplified. It is, however, better not to do so because the ν summation of Eq. (14), as such, converges much faster as was emphasized in Ref. [12]. When $r<a$, Eq. (15) is not necessarily satisfied.

Equations (12) and (14) lead to the following simple expression for $\psi(r,t)$,

$$\psi(r,t)=\sum_\nu c_\nu(r)\mathcal{M}(k_\nu,r-a,t)+c_\kappa(r)\mathcal{M}(i\kappa,r-a,t)+c_{\kappa'}(r)\mathcal{M}(i\kappa',r-a,t)+C_\kappa e^{i\kappa^2t}u_\kappa(r), \tag{16}$$

where the summation is over $\nu=\pm1,\pm2,\ldots$. The $\mathcal{M}(k,x,t)$ is defined by

$$\mathcal{M}(k,x,t)=M(k,x,t)+\frac{1}{k}\chi(x,t). \tag{17}$$

Here $\chi(x,t)$ is defined by

$$\chi(x,t)=\frac{e^{i\pi/4}}{2\sqrt{\pi t}}\exp\left(\frac{ix^2}{4t}\right), \tag{18}$$

and $M(k,x,t)$ is the Moshinsky function [13–15] defined by

$$M(k,x,t)=\frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{e^{-i\zeta^2t}e^{i\zeta x}}{\zeta-k}d\zeta. \tag{19}$$

When k is real the authors of Refs. [13–15] replace k by $k-i\epsilon$ where $\epsilon>0$ is infinitesimal. In the work of this paper k corresponds to k_ν with a negative imaginary part or to $i\kappa$ or $i\kappa'$. When $\mathrm{Im}(k)$ is finite, which is always the case in our discussion, ϵ can be ignored. Let us emphasize that the range of the ζ integration is $(-\infty,\infty)$. When $\zeta<0$, $e^{i\zeta x}$ is an incoming wave. The Moshinsky function $M(k,x,t)$ always contains incoming waves and so does the exact wave function $\psi(r,t)$. This is an important difference from the Gamow wave function which we discuss in Sec. IV.

If $\mathrm{Im}(k)<0$, after the ζ integration, $M(k,x,t)$ becomes

$$M(k,x,t)=\frac{1}{2}e^{-ik^2t}e^{ikx}\mathrm{erfc}(y),\ y=e^{-i\pi/4}\frac{x-2kt}{2\sqrt{t}}, \tag{20}$$

where $\mathrm{erfc}(y)=(2/\sqrt{\pi})\int_y^\infty e^{-u^2}du$. For $\mathrm{Im}(k)>0$, we obtain

$$M(k,x,t)=\frac{1}{2}e^{-ik^2t}e^{ikx}[\mathrm{erfc}(y)-2]. \tag{21}$$

For some details that underlie Eqs. (20) and (21), see Appendix A. In the limit of $t\to0$, $M(k,x,t)$ with $\mathrm{Im}(k)<0$ becomes

$$M(k,x,t)\to e^{ikx}\theta(-x), \tag{22}$$

whereas $M(i\kappa,x,t)$ becomes

$$M(i\kappa,x,t)\to-e^{-\kappa x}\theta(x), \tag{23}$$

where $\theta(x)=1(0)$ if $x>0(x<0)$. The above are discontinuous at $x=0$. For $t>0$ they both become smooth functions of x. They satisfy the free time-dependent Schrödinger equation with $r=x$ and $V(r)=0$.

In order to be consistent with the initial wave function $\psi(r,0)$ which is confined to $r<a$, the $\psi(r,t)$ of Eq. (16) has to vanish for $r>a$ at $t=0$. The part that consists of $M(k_\nu,r-a,t)$ obviously conforms to this condition by itself. There are two remaining terms, one with $M(i\kappa,r-a,t)$ and the other with $c_\kappa(r)u_\kappa(r)$. In the limit of $t\to0$ they both become of the form of $e^{-\kappa(r-a)}$ outside the barrier $r>a$. [Recall that $c_\kappa(r)$ is independent of r when $r>a$.] These two terms should cancel for $r>a$. This means that

$$C_\kappa u_\kappa(a)=c_\kappa. \tag{24}$$

We do not impose this relation. It should be automatically satisfied. We illustrate this relation with example II in the next section. Let us add that, while the bound-state component of $\psi(r,t)$ of Eq. (16) with $u_\kappa(r)$ remains as such, the r dependence of the component with $M(i\kappa,r-a,t)$ changes in time.

In the above we assumed that $h(k,r)$ has no essential singularity. This assumption is valid if $r>a$, but is not necessarily valid if $r<a$. In the examples of the next section, we will illustrate that $h(k,r)$ obtains essential singularities when

$r<a$. Such singularities, however, can easily be handled and we can obtain the wave function in the form of a linear combination of Moshinsky functions also for $r<a$.

Once the wave function is obtained we can examine the survival probability $S(t)$ and the nonescape probability $P(t)$, which are, respectively, defined by

$$S(t)=\left|\int_0^\infty \psi^*(r,0)\psi(r,t)dr\right|^2, \tag{25}$$

$$P(t)=\int_0^a |\psi(r,t)|^2 dr. \tag{26}$$

Note that $S(t)\leqslant P(t)$.

III. EXAMPLES

We illustrate the method presented above by means of three examples, I, II, and III. Example I is the one with which the method was briefly illustrated in Refs. [11,12].

A. Example I: δ-function barrier

We assume the potential to be

$$V(r)=\frac{\lambda}{a}\delta(r-a), \quad \lambda>0. \tag{27}$$

Since $V(r)$ has no attractive part, there is no stationary bound state. All stationary scattering states can be obtained explicitly. In numerical illustrations we set $a=1$. For the strength of the δ-function potential we take $\lambda=6$ and 100. These two choices represent typical situations of fast and slow decay processes [6,11].

Let us first summarize relevant results of the stationary scattering problem. The Jost solution $f(k,r)$ of this example is such that

$$e^{-ikr}f(-k,r)=1-\frac{i\lambda}{2ka}[e^{2ik(a-r)}-1]\theta(a-r). \tag{28}$$

This leads to

$$u(k,r)=\frac{1}{k}\left\{\sin kr\ \theta(a-r) + \frac{\sin ka \sin[kr+\eta(k)]}{\sin[ka+\eta(k)]}\theta(r-a)\right\}, \tag{29}$$

where the phase shift $\eta(k)$ is determined from

$$ka\cot(ka+\eta)=\lambda+ka\cot ka. \tag{30}$$

Let us turn to the time-dependent problem. For the wave function at $t=0$ we assume the normalized wave function

$$\psi(r,0)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi r}{a}\right)\theta(a-r), \tag{31}$$

where $n=1,2,\ldots$. This leads to

$$C(k)=\frac{(-1)^n\sqrt{2a}\,n\pi\sin ka}{k(k^2a^2-n^2\pi^2)}. \tag{32}$$

Let us examine $h(k,r)$ of Eq. (13) for $r>a$ and $r<a$, i.e., outside and inside of the repulsive barrier, separately. When we specifically refer to $r>a$ ($r<a$), we denote $h(k,r)$ with $h(k,r>a)[h(k,r<a)]$. We obtain

$$h(k,r>a)=\frac{(-1)^n i\sqrt{2a}\,nka}{(k^2a^2-n^2\pi^2)(ka\cot ka+\lambda-ika)}, \tag{33}$$

which is independent of r. It has poles at k_ν's, which are determined by

$$ka\cot ka+\lambda-ika=0. \tag{34}$$

When $\lambda\gg 1$, we obtain

$$k_\nu\approx\frac{\nu\pi}{a}\left(1-\frac{1}{\lambda}+\frac{1-i\nu\pi}{\lambda^2}\right), \tag{35}$$

where we have ignored terms like $1/\lambda^3$. In the actual calculation, however, we solve Eq. (34) numerically; see Appendix B. The $h(k,r>a)$ has no essential singularity and hence Eqs. (14) and (16) hold. The residue c_ν of the pole of $(2\pi/i)h(k,r>a)$ at k_ν is independent of r and is given by

$$c_\nu=\frac{(-1)^n 2n\pi\sqrt{2a}\,k_\nu}{(k_\nu^2a^2-n^2\pi^2)[(1+\lambda-ik_\nu a)\cot k_\nu a-i-k_\nu a]}. \tag{36}$$

When $r<a$ the situation is somewhat complicated. The $h(k,r<a)$ is given by

$$h(k,r<a)=h(k,r>a)\left\{1-\frac{i\lambda}{2ka}[e^{2ik(a-r)}-1]\right\}, \tag{37}$$

which shares the same set of poles with $h(k,r>a)$. The term $e^{2ik(a-r)}$ of Eq. (37) gives rise to an essential singularity of $h(k,r<a)$ at infinity. Therefore the Mittag-Leffler expansion (14) does not hold for $h(k,r<a)$. When substituted into Eq. (12), however, this part of $h(k,r<a)$ can be rewritten as

$$\int_{-\infty}^{\infty} e^{-ik^2t}e^{ik(r-a)}e^{2ik(a-r)}h(k,r>a)dk = \int_{-\infty}^{\infty} e^{-ik^2t}e^{ik(a-r)}h(k,r>a)dk. \tag{38}$$

Combining the above with the Mittag-Leffler expansion of $h(k,r>a)$ we obtain a linear combination of the $\mathcal{M}(k_\nu,a-r,t)$ for the different k_ν.

By putting the above together we obtain the wave function for $r>a$,

$$\psi(r>a,t)=\sum_\nu c_\nu\mathcal{M}(k_\nu,r-a,t), \tag{39}$$

and for $r<a$,

$$\psi(r<a,t)=\sum_{\nu} c_{\nu}\left[\left(1+\frac{i\lambda}{2k_{\nu}a}\right)\mathcal{M}(k_{\nu},r-a,t) - \frac{i\lambda}{2k_{\nu}a}\mathcal{M}(k_{\nu},a-r,t)\right]. \tag{40}$$

The above can also be written as

$$\psi(r,t)=\sum_{\nu} c_{\nu}[\mathcal{M}(k_{\nu},r-a,t)+N_{-}(k_{\nu},r-a,t)], \tag{41}$$

where

$$N_{\pm}(k,x,t)=\frac{i\lambda}{2ka}[\mathcal{M}(k,x,t)\pm\mathcal{M}(k,-x,t)]\theta(-x). \tag{42}$$

The $\psi(r,t)$ for $t>0$ is continuous at $r=a$ as can be seen from $N_{-}(k,0,t)=0$. Although it is not obvious from Eq. (40) it can be shown that $\psi(0,t)=0$.

The r derivatives of $\psi(r,t)$ are given by

$$\psi'(r,t)=i\sum_{\nu} c_{\nu}\{k_{\nu}[\mathcal{M}(k_{\nu},r-a,t)+N_{+}(k_{\nu},r-a,t)] + \chi(r-a,t)\}, \tag{43}$$

$$\psi''(r,t)=-\sum_{\nu} c_{\nu}\left\{k_{\nu}^2[\mathcal{M}(k_{\nu},r-a,t)+N_{-}(k_{\nu},r-a,t)] + \frac{r-a+2k_{\nu}t}{2t}\chi(r-a,t)\right\}+\frac{\lambda}{a}\delta(r-a)\psi(a,t). \tag{44}$$

It is not difficult to confirm that ψ given above does satisfy Eq. (2). The δ-function part of ψ'' exactly cancels $V\psi$ in the Schrödinger equation.

We show the wave function for a fairly weak barrier in Fig. 1 and for a strong barrier in Fig. 2. In Figs. 1 and 2 we also show wave functions obtained in the $\{k_1,k_{-1}\}$ approximation in which only the pair of poles k_1 and k_{-1} are included. These are the poles with the smallest magnitude of the real part. For the strong barrier case when $\lambda\gg 1$, the wave function has a clear wave-front structure. It drops off sharply as r exceeds vt where $v\approx \mathrm{Re}(k_1)/m\approx 2\pi$. Recall that $2m=1$. Furthermore there are small humps with speeds $2v,3v$, etc., which correspond to the escape of the states with the higher resonance energies. Their amplitudes are small since the initial state contains only small components of them. The system decays extremely slowly as is evident from the wave function inside the barrier being close to the initial state and the small size of the amplitude of the wave function outside the barrier.

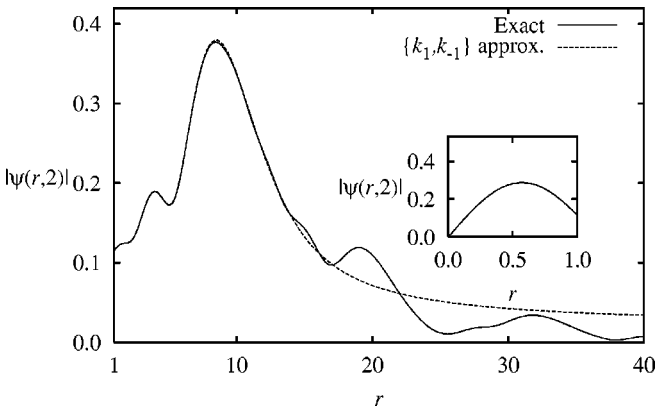

FIG. 1. The modulus of the wave function $|\psi(r,t)|$ for $\lambda=6$, $a=1$ and $t=2$ in example I. The $\{k_1,k_{-1}\}$ approximation includes only the pair of poles, k_1 and k_{-1}, which are the poles with the smallest magnitude of the real part.

B. Example II: Combined δ-function and square-well potential

We assume the potential to be

$$V(r)=\frac{\lambda}{a}\delta(r-a)-D\,\theta(a-r), \qquad \lambda>0, \qquad D>0. \tag{45}$$

Depending on the value of D there can be one or more stationary bound states. We assume that there is only one or no bound state. For the stationary scattering states, the Jost solution $f(k,r)$ is such that

$$e^{-ikr}f(-k,r)=\theta(r-a)+\frac{1}{2}\left[\left(1-\frac{k}{q}-\frac{i\lambda}{qa}\right)e^{iq(a-r)} + \left(1+\frac{k}{q}+\frac{i\lambda}{qa}\right)e^{-iq(a-r)}\right] \times e^{ik(a-r)}\theta(a-r), \tag{46}$$

where

$$q=k\sqrt{1+(D/k^2)}. \tag{47}$$

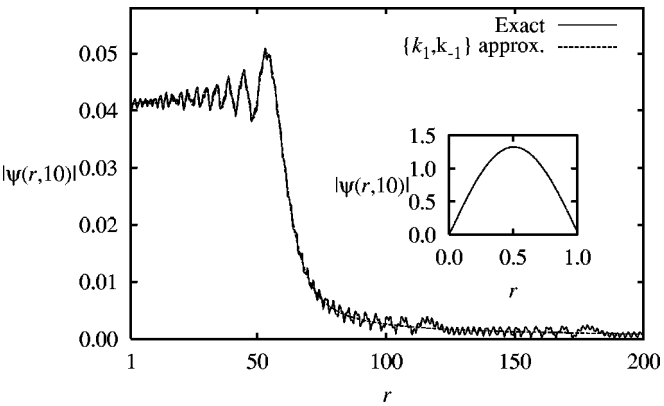

FIG. 2. The modulus of the wave function $|\psi(r,t)|$ for $\lambda=100$, $a=1$, and $t=10$ in example I. For the $\{k_1,k_{-1}\}$ approximation, see the caption of Fig. 1.

For the wave function of the decay problem, we assume the initial condition, Eq. (31). This leads to

$$C(k)=\frac{(-1)^n\sqrt{2a}\,n\pi\sin qa}{q(q^2a^2-n^2\pi^2)}, \tag{48}$$

$$h(k,r>a)=\frac{(-1)^n i\sqrt{2a}\,nka}{(q^2a^2-n^2\pi^2)(qa\cot qa+\lambda-ika)}. \tag{49}$$

The pole position k_ν can be determined by

$$qa\cot qa+\lambda-ika=0. \tag{50}$$

The $h(k,r>a)$ has no singularity other than simple poles. The residue c_ν of $(2\pi/i)h(k,r>a)$ is independent of r and is given by

$$\begin{aligned} c_\nu&=\frac{(-1)^{n-1}2n\pi\sqrt{2a}\,k_\nu q_\nu}{(q_\nu^2a^2-n^2\pi^2)[(1+\lambda-ik_\nu a)k_\nu\cot q_\nu a-(i+k_\nu a)q_\nu]}\\ &=\frac{(-1)^n 2n\pi\sqrt{2a}\,k_\nu q_\nu^2a^2}{(q_\nu^2a^2-n^2\pi^2)[k_\nu a(\lambda-ik_\nu a)(1+\lambda-ik_\nu a)+(i+k_\nu a)q_\nu^2a^2]}, \end{aligned} \tag{51}$$

where $q_\nu=k_\nu\sqrt{1+(D/k_\nu^2)}$.

The case of $r<a$ can be handled in a manner similar to the corresponding case of example I. The $h(k,r<a)$ and $h(k,r>a)$ are related by

$$\begin{aligned} h(k,r<a)=h(k,r>a)\times\frac{1}{2}\Bigg[&\left(1-\frac{k}{q}-\frac{i\lambda}{qa}\right)e^{i(k+q)(a-r)}\\ &+\left(1+\frac{k}{q}+\frac{i\lambda}{qa}\right)e^{i(k-q)(a-r)}\Bigg]. \end{aligned} \tag{52}$$

When $|k|\to\infty, k-q\to 0$. The term $e^{i(k+q)(a-r)}$ of Eq. (52), however, gives rise to an essential singularity of $h(k,r<a)$ at infinity. When substituted into Eq. (12), this part of $h(k,r<a)$ goes like

$$\begin{aligned} &\int_{-\infty}^{\infty}e^{-ik^2t}e^{ik(r-a)}e^{i(k+q)(a-r)}h(k,r>a)dk\\ &\quad=\int_{-\infty}^{\infty}e^{-ik^2t}e^{ik(a-r)}e^{-i(k-q)(a-r)}h(k,r>a)dk. \end{aligned} \tag{53}$$

The positions of the poles are common between $h(k,r<a)$ and $h(k,r>a)$.

Let us now turn to the stationary bound state, which emerges when the **S** matrix has a pole on the positive imaginary axis $k=i\kappa$ where $\kappa>0$. This is the case if

$$q_\kappa a\cot q_\kappa a+\lambda+\kappa a=0, \qquad q_\kappa=\sqrt{D-\kappa^2} \tag{54}$$

is satisfied. If D is sufficiently large, this equation can have one root. Let us calculate C_κ of Eq. (11). The wave function of the bound state is given by

$$u_\kappa(r)=N[\sin q_\kappa r\;\theta(a-r)+e^{-\kappa(r-a)}\sin q_\kappa a\;\theta(r-a)]. \tag{55}$$

The normalization factor N is given by

$$N^{-2}=\frac{1}{2}\left[a+\sin q_\kappa a\left(\frac{\sin q_\kappa a}{\kappa}-\frac{\cos q_\kappa a}{q_\kappa}\right)\right]. \tag{56}$$

The coefficient C_κ is given by

$$C_\kappa=-N\frac{(-1)^n\sqrt{2a}\,\pi\sin q_\kappa a}{q_\kappa^2a^2-n^2\pi^2}. \tag{57}$$

The residue c_κ of $h(k,r>a)$ for the bound-state pole is independent of r and is given by Eq. (51) with $q_\nu=q_\kappa$ and $k_\nu=i\kappa$. With the understanding that $u_\kappa(a)=N\sin q_\kappa a$, a little algebra confirms that Eq. (24) is indeed satisfied.

The wave function $\psi(r,t)$ which starts with the $\psi(r,0)$ of Eq. (31) is given, for $r>a$, by

$$\psi(r>a,t)=\sum_\nu c_\nu\mathcal{M}(k_\nu,r-a,t)+C_\kappa e^{i\kappa^2t}u_\kappa(r). \tag{58}$$

Here and in the following the summation over the **S**-matrix poles includes those on the imaginary axis which lead to terms such as $c_\kappa(r)\mathcal{M}(i\kappa,r-a,t)$ and $c_{\kappa'}(r)\mathcal{M}(i\kappa',r-a,t)$. For $r<a$ we obtain

$$\begin{aligned} \psi(r<a,t)=\frac{1}{2}\sum_\nu c_\nu\Bigg[&\left(1+\frac{k_\nu}{q_\nu}+\frac{i\lambda}{q_\nu a}\right)e^{i(k_\nu-q_\nu)(a-r)}\\ &\times\mathcal{M}(k_\nu,r-a,t)\\ &+\left(1-\frac{k_\nu}{q_\nu}-\frac{i\lambda}{q_\nu a}\right)e^{-i(k_\nu-q_\nu)(a-r)}\\ &\times\mathcal{M}(k_\nu,a-r,t)\Bigg]+C_\kappa e^{i\kappa^2t}u_\kappa(r). \end{aligned} \tag{59}$$

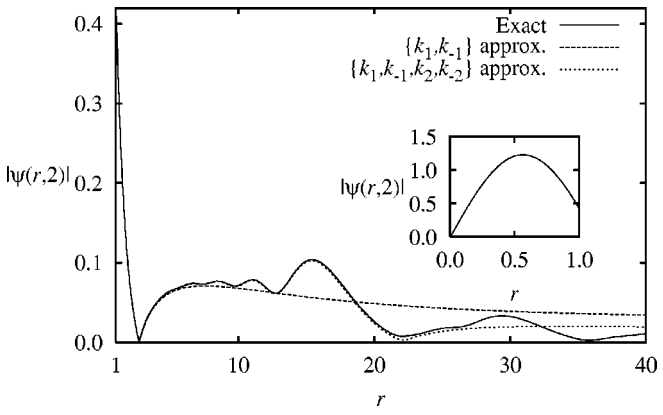

FIG. 3. The modulus of the wave function $|\psi(r,t)|$ for $\lambda=6$, $D=10$, $a=1$, and $t=2$ in example II. This system supports a single bound state with $\kappa=1.4964$.

If there is no bound state, the terms involving κ should be dropped. The above is not a simple superposition of the Moshinsky functions in the sense that the coefficients are not constants.

In Fig. 3 we display the wave function of a decaying system when the system supports a bound state. The $\{k_1,k_{-1},k_2,k_{-2}\}$ approximation includes only the poles k_1,k_{-1},k_2, and k_{-2}.

C. Example III: Square-well plus square-barrier potential

In this example we replace the δ-function barrier of example II with a square barrier of height H,

$$V(r)=H\theta(a-r)\,\theta(r-b)-D\,\theta(b-r), \tag{60}$$

where $H>0,D>0$, and $a>b$. The potential shape is shown in Fig. 4; $c=a-b$ is the width of the repulsive square barrier.

The Jost solution is such that

$$e^{-ikr}f(-k,r)=\theta(r-a)+\frac{1}{2}\left[\left(1-\frac{k}{p}\right)e^{ip(a-r)}+\left(1+\frac{k}{p}\right)e^{-ip(a-r)}\right]\times e^{ik(a-r)}\theta(a-r)\,\theta(r-b)+\frac{1}{4}\left\{\left[\left(1-\frac{k}{p}\right)\times\left(1+\frac{p}{q}\right)e^{ipc}+\left(1+\frac{k}{p}\right)\left(1-\frac{p}{q}\right)e^{-ipc}\right]\times e^{iq(b-r)}+\left[\left(1-\frac{k}{p}\right)\left(1-\frac{p}{q}\right)e^{ipc}+\left(1+\frac{k}{p}\right)\times\left(1+\frac{p}{q}\right)e^{-ipc}\right]e^{-iq(b-r)}\right\}e^{ik(a-r)}\theta(b-r), \tag{61}$$

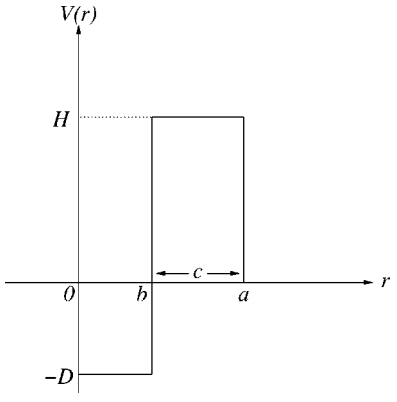

FIG. 4. The potential of example III with the parameters shown.

where q is defined by Eq. (47) and $p=k\sqrt{1-(H/k^2)}$. It is understood that k becomes purely imaginary when $k^2<H$. For $u(k,r)$ we obtain

$$u(k,r)=\frac{1}{q}\sin qr\;\theta(b-r)+\left[\frac{1}{p}\cos qb\sin pc+\frac{1}{q}\sin qb\cos pc\right]\frac{\sin[kr+\eta(k)]}{\sin[ka+\eta(k)]}\,\theta(r-a)+\left[\frac{1}{p}\cos qb\sin p(r-b)+\frac{1}{q}\sin qb\cos p(r-b)\right]\times\theta(a-r)\,\theta(r-b). \tag{62}$$

The phase shift $\eta(k)$ is determined by

$$k\cot(ka+\eta)=\frac{q\cot qb-p\tan pc}{(q/p)\cot qb+1}. \tag{63}$$

In the limits of $c\to 0$ and $Hc\to\lambda/a$, we have $q/p\to 0$ and $p\tan pc\to\lambda/a$.

We assume the same initial condition as Eq. (31) except that we replace a with b. Then $C(k)$ is given by Eq. (48) with a replaced with b. The function $h(k,r>a)$ for $r>a$ is given by

$$h(k,r>a)=\frac{(-1)^n i\sqrt{2b}\,kbe^{ikc}}{(q^2b^2-n^2\pi^2)F(k)}, \tag{64}$$

where

$$F(k)=\frac{a}{p\sin qa}[q\cos qb(p\cos pc-ik\sin pc)-p\sin qb(p\sin pc+ik\cos pc)]. \tag{65}$$

When $c\to 0,F(k)$ is reduced to $qa\cot qa+\lambda-ika$. The pole position k_ν of $h(k,r>a)$ can be determined by $F(k)=0$. The $h(k,r>a)$ has no singularity other than simple poles. The residue c_ν is independent of r and is given by

$$c_\nu=\frac{(-1)^n 2\pi\sqrt{2b}\,k_\nu b}{(q_\nu^2b^2-n^2\pi^2)}\,\frac{e^{ik_\nu c}}{dF(k_\nu)/dk}, \tag{66}$$

where $p_\nu=k_\nu\sqrt{1-(H/k_\nu^2)}$ and $q_\nu=k_\nu\sqrt{1+(D/k_\nu^2)}$.

Next let us turn to $h(k,a>r>b)$ which is related to $h(k,r>a)$ by

$$h(k,a>r>b)=h(k,r>a)\times\frac{1}{2}\left[\left(1-\frac{k}{p}\right)e^{ip(a-r)}+\left(1+\frac{k}{p}\right)e^{-ip(a-r)}\right]e^{ik(a-r)}. \quad (67)$$

The part with $e^{i(k+p)(a-r)}$ has an essential singularity at infinity. We rewrite this as $e^{-i(k-p)(a-r)}e^{2ik(a-r)}$ and do a manipulation similar to Eqs. (38) and (40).

For $h(k,b>r)$ we obtain

$$h(k,b>r)=h(k,r>a)\times\frac{1}{4}\left\{\left[\left(1-\frac{k}{p}\right)\left(1+\frac{p}{q}\right)e^{ipc}+\left(1+\frac{k}{p}\right)\times\left(1-\frac{p}{q}\right)e^{-ipc}\right]e^{iq(b-r)}+\left[\left(1-\frac{k}{p}\right)\times\left(1-\frac{p}{q}\right)e^{ipc}+\left(1+\frac{k}{p}\right)\left(1+\frac{p}{q}\right)e^{-ipc}\right]\times e^{-iq(b-r)}\right\}e^{ik(a-r)}. \quad (68)$$

Each of the combinations of the exponential factors other than the last one, i.e., $e^{-ipc}e^{-iq(b-r)}e^{ik(a-r)}$, gives rise to an essential singularity at infinity.

The wave function $\psi(r,t)$ which starts with the $\psi(r,0)$ of Eq. (31) with a replaced by b is given, for $r>a$, by

$$\psi(r>a,t)=\sum_\nu c_\nu\mathcal{M}(k_\nu,r-a,t)+C_\kappa e^{i\kappa^2 t}u_\kappa(r). \quad (69)$$

Here and in the following the summation over the **S**-matrix poles includes those on the imaginary axis, if any, which leads to terms such as $c_\kappa(r)\mathcal{M}(i\kappa,r-a,t)$ and $c_{\kappa'}(r)\mathcal{M}(i\kappa',r-a,t)$.

For $a>r>b$ we obtain

$$\psi(a>r>b,t)=\frac{1}{2}\sum_\nu c_\nu\times\left[\left(1+\frac{k_\nu}{p_\nu}\right)e^{i(k_\nu-p_\nu)(a-r)}\times\mathcal{M}(k_\nu,r-a,t)+\left(1-\frac{k_\nu}{p_\nu}\right)\times e^{-i(k_\nu-p_\nu)(a-r)}\mathcal{M}(k_\nu,a-r,t)\right]+C_\kappa e^{i\kappa^2 t}u_\kappa(r). \quad (70)$$

For $b>r$ we obtain

$$\psi(b>r,t)=\frac{1}{4}\sum_\nu c_\nu\left[\left(1+\frac{k_\nu}{p_\nu}\right)\left(1+\frac{p_\nu}{q_\nu}\right)e^{-i[p_\nu c+q_\nu(b-r)]}\times\mathcal{M}(k_\nu,r-a,t)+\left(1-\frac{k_\nu}{p_\nu}\right)\left(1+\frac{p_\nu}{q_\nu}\right)e^{i[p_\nu c+q_\nu(b-r)]}\times\mathcal{M}(k_\nu,a-r,t)+\left(1+\frac{k_\nu}{p_\nu}\right)\left(1-\frac{p_\nu}{q_\nu}\right)\times e^{i[-p_\nu c+q_\nu(b-r)+k_\nu(a-2b+r)]}\mathcal{M}(k_\nu,b-r,t)+\left(1-\frac{k_\nu}{p_\nu}\right)\left(1-\frac{p_\nu}{q_\nu}\right)e^{i[p_\nu c-q_\nu(b-r)-k_\nu(a-2b+r)]}\times\mathcal{M}(k_\nu,a-b,t)\right]+C_\kappa e^{i\kappa^2 t}u_\kappa(r). \quad (71)$$

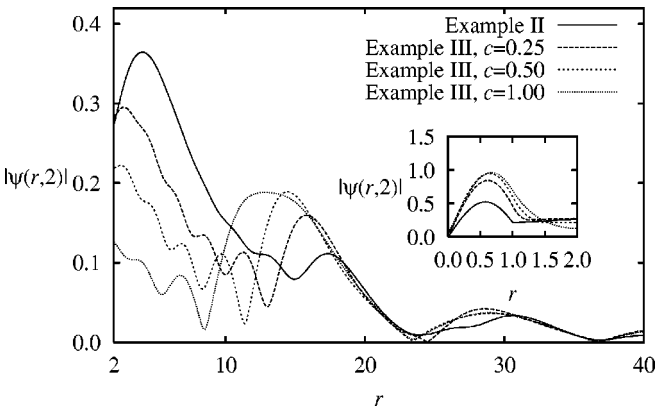

FIG. 5. The modulus of the wave function $|\psi(r,t)|$ when $t=2$ for $\lambda=6$, $a=1$, and $D=5$ of example II, and for $\lambda=Hc$, $D=5$, $b=1$, and $c=0.25$,0.5, and 1.0 in example III.

The results obtained above can be generalized to the case in which the potential $V(r)$ has many steps. We will do this in Appendix C.

The wave function for example III is displayed in Fig. 5 for barriers of different widths and compared with the wave function for the zero-width barrier of example II. We consider a few different values of the barrier width c but keep the ''area'' of the repulsive barrier the same, i.e., $Hc=\lambda$ with $\lambda=6$.

The behavior of the wave function, at times which differ by orders of magnitude, is shown in Fig. 6 and Fig. 7. In Fig. 6 the barrier is a fairly weak one and at $t=10$ the largest part of the wave function exists outside the barrier although there is still a finite probability of finding the particle inside the barrier. At $t=100$ and $t=1000$ the particle has almost com-

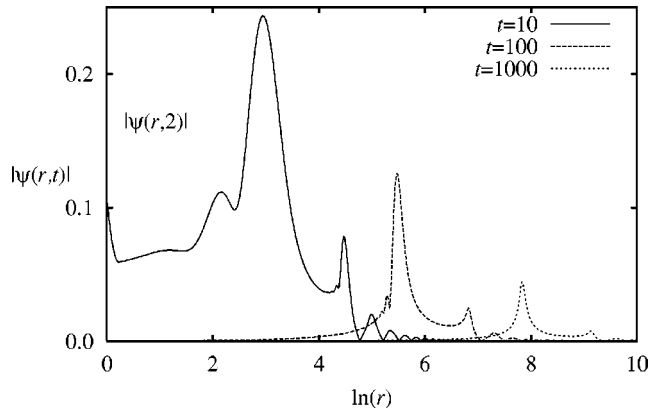

FIG. 6. The modulus of the wave function $|\psi(r,t)|$ for $D=5$, $H=24$, $b=1$, and $c=0.25$ in example III.

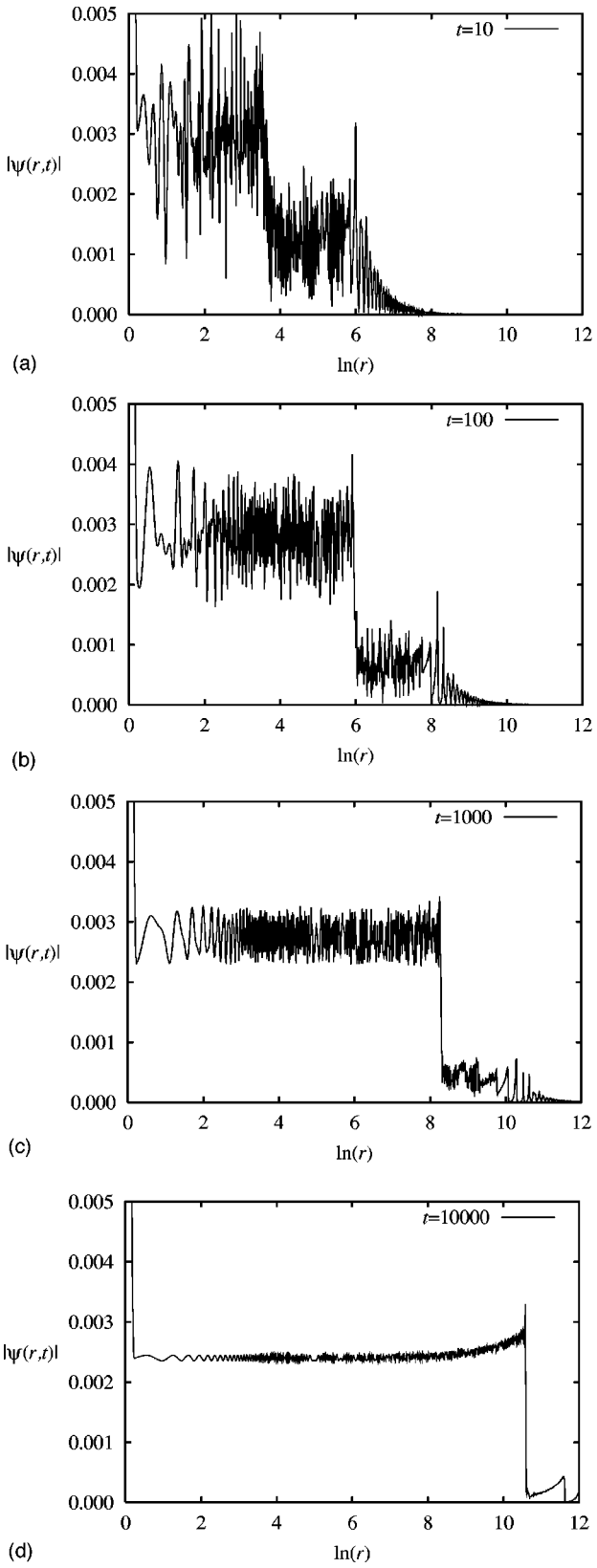

FIG. 7. The modulus of the wave function $|\psi(r,t)|$ for $D=5$, $H=400$, $b=1$, and $c=0.25$ in example III.

pletely escaped the system and propagates as a wave packet with constant speed. The peaks of the wave packets occur almost precisely at

$$r=vt, \qquad v=2\sqrt{\pi^2-D}. \tag{72}$$

The $v^2/4$ is the energy of the system at $t=0$. Recall that $2m=1$. With $D=5$, we obtain $v=4.413$.

The system considered in Fig. 7 is one with a strong barrier and a very long half-life. The striking feature is that the amplitude of the outgoing wave increases exponentially as a function of r and it drops sharply at a ''wave front.'' The drops occur at the same values of r as the peaks in Fig. 6. This can be attributed to the fact that we used the same initial state in both cases so that the energy composition of the initial wave packet is the same in both cases. The wave function of Fig. 7 becomes more regular as time increases. Preceding the main wave front there is a miniature replica of the same shape. This is due to higher energy resonance states which are contained in the initial wave function with much smaller amplitude.

In Ref. [11] we proposed a heuristic form for the wave function of a slowly decaying system, which we subsequently employed in a model study of the atomic ionization following the α decay of the nucleus [16]. The form of the proposed wave function is, for $r>a$,

$$\phi(r,t)=\sqrt{\frac{\Gamma}{v}}e^{i\gamma}e^{-\Gamma/2(t-r/v)}e^{-i[k^2-(\Gamma/4k)^2]t}e^{ikr}\theta\left(t-\frac{r}{v}\right), \tag{73}$$

where Γ is the width of the decaying state, $k=v/2$, and v is the speed defined by Eq. (72). The constant phase factor $e^{i\gamma}$ is related to the choice of the initial wave function. This is a good approximation based on studies with the δ-function potential. The graph of Fig. 7 indicates that the wave function of a potential with a barrier of finite width is also well described by this function especially after a long time. At $t=10^4$, the main wave front has traveled $r\sim 4.4\times 10^4$, which, if $r=1$ is the nuclear radius, is of the order of magnitude of the atomic radius. Thus the above $\phi(r,t)$ is an appropriate wave function for the study of atomic ionization due to α decay [16]. Note that the strength of the potential that we are assuming is such that it gives a half-life which is much smaller than those of the known α emitting nuclei. If we increase the strength of the potential barrier so that the decay half-life becomes more realistic, $\phi(r,t)$ will become an even better approximation.

IV. THE GAMOW WAVE FUNCTION

Let us examine the Gamow wave function [17–20] by focusing on its behavior outside the barrier $r>a$. The Gamow wave function, $\psi_G(r,t)$, is an eigenstate of the Hamiltonian

$$\hat{H}=-(\partial^2/\partial r^2)+V(r). \tag{74}$$

It is subject to two boundary conditions. The first one is $\psi_G(0,t)=0$. The second one is that, outside the barrier r

$>a$, it consists of outgoing waves only. The latter condition cannot be satisfied unless the energy eigenvalue is complex.

The $\psi_G(r,t)$ can be related to the scattering solution of Eqs. (3) and (4) as follows. When $r>a$,$u(k,r)$ takes the form

$$u(k,r)\propto \mathbf{S}(k)e^{ikr}-e^{-ikr}, \tag{75}$$

where $\mathbf{S}(k)$ is the $\mathbf{S}$ matrix. If $k=k_1$ where k_1 is one of the poles of the $\mathbf{S}$ matrix, $\mathbf{S}(k_1)=\infty$ and $u(k_1,r)\propto e^{ik_1 r}$ for $r>a$ and the second boundary condition is satisfied. Thus we obtain

$$\psi_G(r,t)\propto e^{-ik_1^2 t}u(k_1,r). \tag{76}$$

Since $\mathrm{Im}(k_1)<0$, the amplitude of $\psi_G(r,t)$ grows exponentially as r increases. This wave function is not normalizable in the usual sense [17–21,29].

The $\psi_G(r,t)$ satisfies the time-dependent Schrödinger equation (2) but not the initial condition with given $\psi(r,0)$. The $\psi_G(r,t)$ represents a state such that the decay process started at $t=-\infty$ and it has been going on in a *stationary* manner. This is why the wave function is not normalizable [17,29]. The $\psi_G(r,t)$ has no memory as to how and when the decay process started.

The exact wave function that we have constructed is not an eigenfunction of $\hat{H}$. It consists of the Moshinsky functions $M(k,x,t)$. As we emphasized below Eq. (19), $M(k,x,t)$ is a superposition of incoming and outgoing waves. Each of the Moshinsky functions involved has a wave front and is square integrable. Our wave function is always normalized to unity. For the normalizability, the presence of the incoming waves is essential.

A technique to expand the wave function in terms of Gamow-type wave functions has been developed; see, e.g., Ref. [20]. However, the fact that the exact wave function contains incoming waves at the boundary $r=a$ implies that such an expansion is not possible in a strict sense. The outgoing wave component is much larger than the incoming wave component in general. Therefore such an expansion is usually a good approximation but it cannot be exact. We will see a relevance of this aspect in the next section.

V. ASYMPTOTIC BEHAVIOR OF THE SURVIVAL AND NONESCAPE PROBABILITIES

In this section we are interested in the behavior of the survival probability $S(t)$ and the nonescape probability $P(t)$ as functions of t when $t\to\infty$. We assume that there is no stable bound state with κ in this section until towards the end. García-Caldéron, Mateos, and Moshinsky [22,23] examined these probabilities for a decaying system and stated that $S(t)$ and $P(t)$ obey different power laws after long times, i.e., $S(t)\sim t^{-3}$ and $P(t)\sim t^{-1}$. Recall that $S(t)\leqslant P(t)$ in general. In a comment on Ref. [22], Cavalcanti [25] showed that $S(t)$ and $P(t)$ both vary as t^{-3} as $t\to\infty$. García-Caldéron *et al.* [24] responded that Cavalcanti evaluated $P(t)$ by taking the long-time limit prior to integrating over r, whereas reversing the order of the operations leads to a t^{-1} long-time behavior. The issue is not settled. These analyses involved the expansion of the wave function in terms of Gamow resonance states.

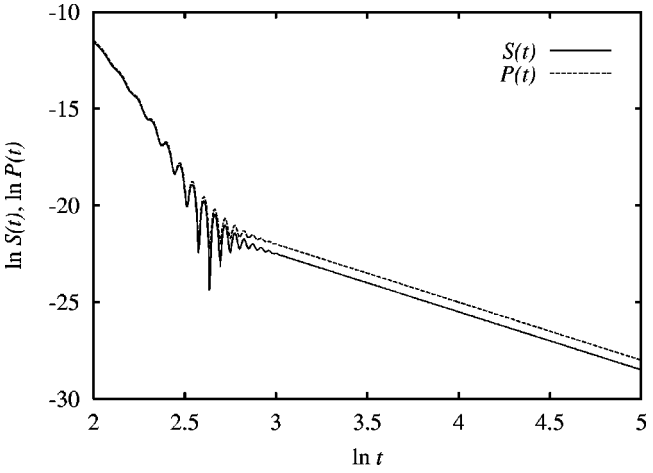

FIG. 8. The survival and nonescape probabilities plotted as functions of t, in a log-log scale, for the δ-shell potential of example I with $\lambda=6$ and $a=1$.

Let us reexamine this problem by means of our examples. As we have shown in the preceding sections, the wave function $\psi(r,t)$ can be expressed in the form of a linear combination of $\mathcal{M}(k_\nu,x,t)$ where x is of the form of $x=\pm r+\text{const}$. When $t\to\infty$ the Moshinsky function $M(k,x,t)$ becomes

$$M(k_\nu,x,t)\to -\frac{e^{i(\pi+x^2/t)/4}}{2\sqrt{\pi}}\frac{1}{k_\nu\sqrt{t}}\left(1-\frac{i}{2k_\nu^2 t}-\frac{3}{4k_\nu^4 t^2}+\cdots\right). \tag{77}$$

In the $\mathcal{M}(k,x,t)$ of Eq. (17), the leading term of $M(k,x,t)$ proportional to $1/\sqrt{t}$ is exactly canceled by the added term of $(1/k)\chi(x,t)$. It then follows that $\mathcal{M}(k,x,t)\sim t^{-3/2}$ as $t\to\infty$.

If there is no bound state, the $\psi(r,t)$ for very large values of t becomes

$$\psi(r,t)\sim t^{-3/2} \qquad \text{as} \quad t\to\infty. \tag{78}$$

This holds for any value of r and for any of the examples that we have examined. Thus we find that $S(t)$ and $P(t)$ both vary as t^{-3} as $t\to\infty$. Figure 8 shows the behavior of the survival and nonescape probabilities as functions of time for a particular case of example I.

In Fig. 9 we show $S(t)$ and $P(t)$ of example II with $\lambda=6$, $D=5$, and $a=1$. With this value of D there is no stationary bound state. The two probabilities again vary as t^{-3} at large times. Oscillations of both probabilities occur in the transition region where the exponential decay changes into a power-law behavior. In calculating the $S(t)$ and $P(t)$, we used the exact evaluation of $\psi(r,t)$ at all values of t. Contrary to the remark of García-Caldéron *et al.* [24], the order of the operations of integrating over r and letting t become large is irrelevant in our calculation.

It should be noted that in our calculations both $S(t)$ and $P(t)$ fluctuate as a function of time when these quantities

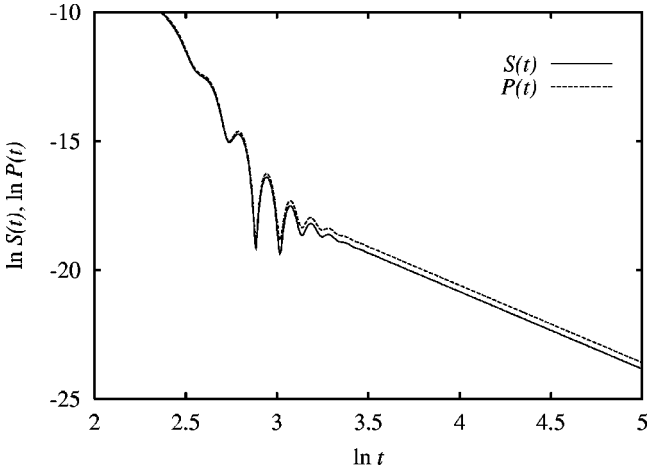

FIG. 9. The nonescape and survival probabilities plotted as functions of t, in a log-log scale, for the potential of example II with $\lambda=6$, $D=5$, and $a=1$.

make the transition from the exponential decay law to the power-of-t decay law. This feature of quantum decaying systems was first pointed out by Winter [5]. In Refs. [22,23] only $S(t)$ shows the fluctuations while $P(t)$ makes a smooth transition from one region in time to the other. This is because, as we pointed out in Sec. IV, the wave function that was used in Ref. [22] has no incoming wave component at and outside the potential barrier. In contrast the exact wave function always contains incoming waves. Cavalcanti [25] obtained the correct t^{-3} behavior of $P(t)$, but used the same inexact expansion of the wave function as that of Ref. [22], and hence his analysis is incomplete.

So far we have assumed that there is no stationary bound state. Let us consider example II with a bound state of energy $-\kappa^2$. The wave function has the bound-state term $C_\kappa e^{i\kappa^2 t}u_\kappa(r)$. In the limit of $t\to\infty$, all other terms with Moshinsky functions are dispersed in the entire space. In this sense $\psi(r,t)\to C_\kappa e^{i\kappa^2 t}u_\kappa(r)$. The probabilities $P(t)$ and $S(t)$, respectively, approach finite constant values,

$$S(\infty)=|C_\kappa|^2\left|\int_0^\infty \psi^*(r,0)u_\kappa(r)dr\right|^2, \tag{79}$$

$$P(\infty)=|C_\kappa|^2\int_0^a |u_\kappa(r)|^2 dr. \tag{80}$$

The differences $S(t)-S(\infty)$ and $P(t)-P(\infty)$ both behave as t^{-3} as t becomes very large.

The deviation from the exponential law for very small values of t is an interesting subject. We examined it in considerable detail for example I in Ref. [12]. The situations for examples II and III are similar to that of example I.

VI. DISCUSSION

We have presented a full account of an analytical method of solving the time-dependent Schrödinger equation for a model that simulates the nuclear α decay. For the potential for the α particle we assumed a potential that is piecewise constant. The method is such that, if one knows all the solutions for stationary states analytically, one can obtain the solution of the time-dependent Schrödinger equation in the form of a linear combination of the Moshinsky functions.

Since the method is analytical, one can obtain the solution regardless of the magnitudes of r and/or t. This is an important advantage of the method over purely numerical methods. Our method will enable us to examine various features of slow decay processes. One such example is the deviation from the exponential law for very large times, which we discussed in Sec. V. All the results presented in this paper, except for the deviation from the exponential decay law at very large times, were confirmed by numerically solving the time-dependent Schrödinger equation. This gives us full confidence in our analytical method.

Mişicu *et al.* [9] considered a model that simulates the α decay of ^{212}Po. For the ground state of their model, $E_\alpha=8.88$ MeV and the decay half-life is $T_{1/2}=1.5\times10^{-9}$ s. They show the time development of the system up to $t=3\times10^{-20}$ s, which is $2\times10^{-11}T_{1/2}$. In order to be able to see interesting features of the decaying system, one would like to solve the time-dependent Schrödinger equation at least up to $t\approx T_{1/2}$. It is prohibitive to do so by numerical integration of the time-dependent Schrödinger equation. Mişicu *et al.* also considered an excited state with $E_\alpha=19.3$ MeV and $T_{1/2}=4.5\times10^{-21}$ s. In this case they presented results up to $t=5\times10^{-21}$ s which is as large as the $T_{1/2}$. This case, however, is one for which no experimental data are available. In cases for which there are experimental data, the initial state of the α particle is one of the lowest energy states.

We pointed out an important difference between our exact wave function and the Gamow wave function. The latter has only outgoing waves outside the barrier. Our wave function contains incoming waves. This difference is related to the fact that the Gamow wave function is not normalizable in the usual sense whereas our wave function remains normalized to unity throughout. The Gamow wave function has no memory about the beginning of the decay process. The presence of the incoming wave component in the exact wave function manifests itself through the fluctuations of the nonescape probability $P(t)$ in the transition time region from the exponential law behavior to the power-law behavior.

The method that we have developed has a few conceivable extensions. A potential of an arbitrary form can be approximated by a potential with many steps. We briefly discussed such a case in Appendix C. In the beginning of Sec. II we stated: "We assume a central potential $V(r)$ such that it has a repulsive barrier which supports one or more unstable bound states or resonances." The method, however, can handle potentials of different forms, e.g., an attractive square-well potential. We assumed the initial wave function $\psi(r,0)$ that is confined within $r<a$. This restriction can be easily removed. For example, we can start with a wave packet that is incident towards the "nucleus." Thus in principle this approach can be used for a time-dependent analysis of the scattering problem.

Having developed the method for the S wave decay, we surmise that it is fruitful to consider higher partial wave decay situations. Furthermore since the Jost functions for po-

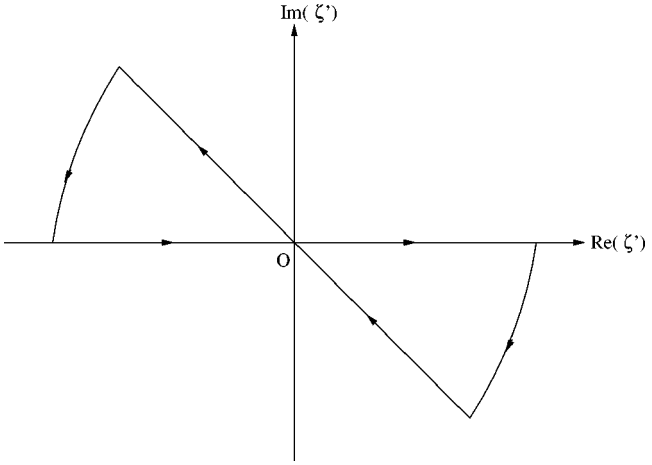

FIG. 10. The integration contour in the complex ζ' plane.

tentials which do not have a sharp boundary and the analogue of the Jost functions for the Coulomb potential are known [30], exploration of the method with such potentials may give further insight into the decay and scattering problems. The Coulomb potential is important in α decay and ways of combining it with a potential well would be important to study details of more realistic α decay.

ACKNOWLEDGMENTS

This work was supported by the Natural Sciences and Engineering Research Council of Canada.

APPENDIX A: THE MOSHINSKY FUNCTION

We need the Moshinsky function $M(k,x,t)$ with k that corresponds to the poles of the **S** matrix, i.e., $k_\nu, i\kappa(\kappa>0)$, or $i\kappa'(\kappa'<0)$. It is convenient to change the integration variable from ζ to $\zeta'=\zeta-(x/2t)$. Then $M(k,x,t)$ becomes

$$M(k,x,t)=\frac{i}{2\pi}e^{ix^2/(4t)}\int_{-\infty}^{\infty}\frac{e^{-i\zeta'^2 t}}{\zeta'-\left(k-\frac{x}{2t}\right)}d\zeta'. \quad \text{(A1)}$$

By using the contour in the complex ζ' plane shown in Fig. 10 and setting

$$\zeta'=e^{-i\pi/4}\frac{s}{\sqrt{t}}, \qquad z=-iy=-e^{i\pi/4}\frac{x-2kt}{2\sqrt{t}}, \quad \text{(A2)}$$

we obtain

$$M(k,x,t)=\frac{i}{2\pi}e^{ix^2/(4t)}\int_{-\infty}^{\infty}\frac{e^{-s^2}ds}{s-z}+\sigma e^{-ik^2 t}e^{ikx}, \quad \text{(A3)}$$

where the last term on the right hand side is determined by the position of the pole at $k-x/(2t);\sigma=1$ if the pole lies inside the contour in the fourth quadrant, $\sigma=-1$ if it lies inside the contour in the second quadrant, and $\sigma=0$ otherwise. The s integration can be done with the result [31]

$$\int_{-\infty}^{\infty}\frac{e^{-s^2}ds}{s-z}=-i\pi e^{y^2}\begin{cases}\mathrm{erfc}(y)-2 & \text{if } \mathrm{Im}(z)>0,\\ \mathrm{erfc}(y) & \text{if } \mathrm{Im}(z)<0.\end{cases} \quad \text{(A4)}$$

Combining the above results we obtain Eqs. (20) and (21).

APPENDIX B: DETERMINATION OF THE S-MATRIX POLES AND PERFORMING SUMMATIONS

In order to solve the nonlinear Eqs. (34) and (50) and $F(k)=0$ where $F(k)$ is given by Eq. (65) for their complex roots, we use the Muller method [32]. The poles and residues need to be calculated only once to determine the wave function of a particular potential at different values of r and t. Given a convergence criterion for the series of the wave function, different numbers of terms are required to obtain $\psi(r,t)$ at different values of r and t. Therefore we initially evaluate more than the maximum number of poles and residues required. The Muller method, like other fixed-point iterative procedures, requires initial guesses and so we start with the poles with the largest magnitude since, according to Ref. [27], as $\nu\to\infty$,

$$\mathrm{Re}(k_\nu)=\nu\pi/a+O(1), \quad \text{(B1)}$$

$$\mathrm{Im}(k_\nu)\propto\ln\nu+O(1). \quad \text{(B2)}$$

The relation for $\mathrm{Re}(k_\nu)$ is very useful for bracketing the position of the pole. The initial estimate for $\mathrm{Im}(k_\nu)$ can be obtained quickly by trial and error. Once the first pole for some large ν is known, $k_\nu-\pi/a$ is a good initial estimate for the $(\nu-1)$th pole. As we get to poles which are close to the origin some adjustments have to be made to ensure that the iterations do not converge to the same pole twice or skip a pole. For small r and t we have made comparisons of $\psi(r,t)$ calculated using the method of this paper and that obtained by integrating the time-dependent Schrödinger equation directly. When they are identical we are confident that we have the correct set of poles. The poles have been obtained with an absolute and relative error of 10^{-10}. The poles in the fourth quadrant are obtained in this manner, whereas those in the third quadrant are simply obtained by changing the sign of the real part.

For the calculation shown in Fig. 1 we used a stringent condition on the summation so that the magnitude of the last term was less than 10^{-8} times the sum. We define ν_{max} as the max$|\nu|$ needed for a convergent series. For the calculation of example I, min$\nu_{max}=21$ and max$\nu_{max}=318$. The maximum value occurred when the wave function had the smallest magnitude. Fewer terms would have sufficed for the purposes of the graph, and the number could have been reduced further by including an absolute error criterion for the sum as well.

In example I, Eq. (15) is satisfied for both $r<a$ and $r>a$. Simplifying Eq. (14) to exclude the $1/k_\nu$ terms, we also obtain Fig. 1. In this case however min$\nu_{max}=2819$ and max$\nu_{max}=31\,799$. Clearly the rate of convergence is much improved by retaining the $1/k_\nu$ terms. For examples II and III these terms must be included when $r<a$ since Eq. (15) does not hold in those cases.

APPENDIX C: POTENTIAL WITH MANY STEPS

Consider a sequence of positions $0=a_0<a_1<a_2<\cdots<a_J=a$ with which we divide the space into $J+1$ regions including the one for which $r>a$. Assume that $V(r)$ is a constant in each of the regions: $V(r)=0$ for $r>a$, and

$$V(r)=V_j \quad \text{for } a_{j-1}<r<a_j, \tag{C1}$$

where $j=1,2,\ldots,J$.

Let us consider a stationary solution of the Schrödinger equation $\phi(k,r)e^{-ik^2t}$ such that

$$\phi(k,r)=Ae^{ikr}+Be^{-ikr} \quad \text{for } r>a, \tag{C2}$$

$$\phi(k,r)=A_je^{ik_jr}+B_je^{-ik_jr} \quad \text{for } a_{j-1}<r<a_j, \tag{C3}$$

where the coefficients A_j's and B_j's are all constants and

$$k_j=k\sqrt{1-(V_j/k^2)}. \tag{C4}$$

If $A=1$ and $B=0$, then $\phi(k,r)$ becomes the Jost solution $f(-k,r)$. Similarly, $\phi(k,r)=f(k,r)$ if $A=0$ and $B=1$.

For given $A=A_{J+1}$ and $B=B_{J+1}$, A_j and B_j can be determined by repeated applications of the following transformation,

$$\begin{pmatrix} A_{j'} \\ B_{j'} \end{pmatrix}=T_{j'j}\begin{pmatrix} A_j \\ B_j \end{pmatrix}, \tag{C5}$$

$$T_{j'j}=\frac{1}{2}\begin{pmatrix} e^{-ik_{j'}a_{j'}} & 0 \\ 0 & e^{ik_{j'}a_{j'}} \end{pmatrix}\begin{pmatrix} 1+\dfrac{k_j}{k_{j'}} & 1-\dfrac{k_j}{k_{j'}} \\ 1-\dfrac{k_j}{k_{j'}} & 1+\dfrac{k_j}{k_{j'}} \end{pmatrix}\times\begin{pmatrix} e^{ik_ja_{j'}} & 0 \\ 0 & e^{-ik_ja_{j'}} \end{pmatrix}, \tag{C6}$$

where $j'=j-1$ and $k_{J+1}=k$. This enables us to write the Jost solutions $f(\pm k,r)$, Jost functions $f(\pm k)$, and then $h(k,r)$ of Eq. (13) for the model. Example III is a special case with $J=2$, $a_1=b$, $a_2=a$, $V_1=-D$, $V_2=H$, $k_1=q$, and $k_2=p$.

Next let us turn to some details of $h(k,r)$ and the wave function $\psi(r,t)$. Assume the same initial wave function $\psi(r,0)$ as that of Eq. (31). The $h(k,r>a)$ and its residue c_ν are independent of r and $h(k,r>a)$ is a meromorphic function of k. The $\psi(k,r>a)$ is of the same form as Eqs. (16) or (69) except that the residue c_ν is different.

When $r<a$, $h(k,r)=e^{-ikr}f(-k,r)h(k,r>a)$ obtains an essential singularity at infinity. This is because of the exponential factors involved in $e^{-ikr}f(-k,r)$ as we have shown in the examples of Sec. III. There is always one combination of the exponential factors that is harmless, i.e., it does not give rise to an essential singularity to $h(k,r>a)$. This is the one of the form of

$$\exp\{-i[k_j(a_j-r)+k_{j+1}(a_{j+1}-a_j)+\ldots+k_J(a-a_{J-1})]+ik(a-r)\}. \tag{C7}$$

This combination leads to a term with $\mathcal{M}(k_\nu,r-a,t)$ of $\psi(r,t)$ as shown, e.g., in Eqs. (70) and (71). Other combinations can be manipulated such that they lead to terms with $\mathcal{M}(k_\nu,a-r,t)$, etc.

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