Adiabaticity in a time-dependent trap: The passage near a continuum threshold

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We consider a time-dependent trap externally manipulated in such a way that one of its bound states is brought up towards the continuum threshold and then down again. We evaluate the probability P^{stay} of a particle, initially in a bound state of the trap, continuing in it at the end of the passage. We use the Sturmian representation, whereby the problem is reduced to evaluating the reflecting coefficient of an absorbing potential. In the slow-passage limit, P^{stay} goes to 1 for a state turning before reaching the continuum threshold and vanishes if the bound state crosses into the continuum. For a slowly moving state, just "touching" the threshold P^{stay} tends to a universal value of about 38%, for a broad class of potentials. In the rapid-passage limit, P^{stay} depends on the choice of the potential. Various types of trapping potentials are considered, with an analytical solution obtained in the special case of a zero-range well.

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I. INTRODUCTION

Recent technological developments have renewed the interest in the dynamics of a particle, or particles, trapped in bound states of time-dependent potentials. External manipulation of Hamiltonians with both discrete and continuum spectra routinely occur in applications such as metrology and quantum information processing. The presence of a continuum plays an important role in atom lasers [1,2], in the preparation of atomic pulses with a known velocity distribution [3], and in the production of few-body number states [4–10]. Quite often a continuum is responsible for undesirable loss of trapped particles, as happens in transport of trapped ions and in trapped ion atomic clocks. An obvious way to avoid such loss is to manipulate the trapping potential sufficiently slowly (adabatically) so that the trapped particle will remain trapped throughout the evolution.

The question of adiabaticity in bound-to-continuum transitions, studied by various authors [11–14], leaves room for further discussion, even with regard to its formulation. As a trapping potential becomes shallower, a bound state is brought closer to the continuum and, eventually, joins it. With this drastic reorganization of the adiabatic spectrum, application of methods developed for level crossing situations, such as the original Landau-Zener model [15] and its numerous generalizations, is problematic at best. Moreover, in an experimental situation one is likely to control the shape of the trap, so that the evolution of the energy of the bound state near the continuum threshold must be deduced from that of the potential. With this in mind, one may be interested in asking two distinct questions. First, let the depth of the trap decrease linearly with time. When evolution stops, what is the probability of its remaining in the modified bound state? Second, let the depth of the potential first decrease and then increase again, e.g., being a quadratic function of time. What is the probability of its remaining in a bound state at the end of the passage? The first case was studied in [16]. In this paper, we consider the second generic case, where a time-dependent trap is manipulated in such a manner that a bound state completes a passage near the continuum threshold, first rising towards it and then moving away again. There are three possibilities: the state may "turn" and begin the downward part of its journey before reaching the threshold. Alternatively, it can just "touch" the threshold once, or cross into the continuum temporarily, to reappear at a later time. In all cases we want to know the probability of its remaining in the initial state or, more generally, inside the well, once the passage is completed.

As in [16] we employ the Sturmian technique, developed in Refs. [17–20] for applications in the theory of atomic collisions. In this way, we reduce the problem of solving a time-dependent Schrödinger equation (SE) to the simpler problem of determining the reflection coefficient of a complex-valued "potential." This, in turn, will allow us to gain further insight into what happens near a continuum threshold and, occasionally, obtain an exact analytical solution to the problem.

The rest of the paper is organized as follows: in Sec. II we formulate the problem of a time-dependent trap, which can lose a previously bound particle to the continuum. In Sec. III we introduce the Sturmian basis and use it to expand the particle's state. In Sec. VI we consider a zero-range well and formulate the adiabatic condition for the passage. In Sec. V we solve the zero-range problem exactly for the case where the bound state just touches the continuum threshold. We show that the probability of remaining in the well is independent of the rate of change of the potential and always equals approximately 38%. In Sec. VI the general case of a zero-range potential is analyzed. In Sec. VII we consider the Sturmian representation of a rectangular potential and the corresponding adiabatic limit. In Sec. VIII we employ the single-Sturmian approximation in order to describe the particle's evolution in a rectangular well. In Sec. IX we show that the 38% rule introduced in Sec. V applies universally in the slow-passage limit to a wide class of potentials whose evolution is quadratic in time. Section X reports our conclusions.

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II. LOSS AND RECAPTURE OF PARTICLES BY A TIME-DEPENDENT POTENTIAL WELL

We start by considering a particle of mass μ in a one-dimensional potential,

$$V(x,t) = -W(x)\sum_{k=0}^{K} V^{(k)}t^k, \tag{1}$$

where $W(x)$ is normalized by the condition $\int_{-\infty}^{\infty} W(x)dx = 1$. The potential is obtained by varying the magnitude of a finite-range potential well $-W(x) < 0$ by means of a time-dependent factor, so that whenever $\sum_{k=0}^{K} V^{(k)}t^k$ turns negative, $V(x,t)$ becomes a barrier, which does not support bound states. The question we ask is the following one: If a particle is put into one of the bound states of the well, ϕ_n, what is the probability of finding it there at some time in the future? The SE to be solved has the form (we use $\hbar = 1$)

$$i\partial_t \Psi(x,t) = -\partial_x^2\Psi/2\mu + V(x,t)\Psi, \tag{2}$$

and we assume that the potential is a deep well in the distant past and future, $V(x,t) < 0$, for $t \to \pm\infty$. A particle in a bound state $\phi_m(x,t)$, $\langle\phi_m|\phi_m\rangle = 1$ with a large negative energy $E_m(t) < 0$ should remain in it for some time, before approaching the continuum threshold [16]. For $\Psi(x,t)$ in Eq. (3) we, therefore, write

$$\lim_{t\to-\infty} \Psi(x,t) = \exp\left[-i\int^t E_m(t')dt'\right]\phi_n(x,t). \tag{3}$$

Similarly, for $t \to \infty$, we should have

$$\lim_{t\to\infty} \Psi(x,t) = \sum_n A_{mn} \exp\left[-i\int^t E_n(t')dt'\right] \times\phi_n(x,t) + \delta\Psi(x,t), \tag{4}$$

where the first term corresponds to the particles which remain in the well, although possibly not in the same state, and $\delta\Psi$ describes the particles lost to the continuum during the passage.

Thus, the total probability of the particle's remaining in the well is given by

$$P_m^{\text{stay}} \equiv \sum_n P_{mn}^{\text{stay}} = \sum_n |A_{mn}|^2. \tag{5}$$

In the following we consider the simplest case of a passage, which is quadratic in time,

$$V(x,t) = (\mathcal{E} - v^2t^2)W(x), \tag{6}$$

and of a particle trapped in an ascending bound state in the distant past, which may remain trapped in one of the descending states or be ejected into the continuum as $t \to \infty$ (see Fig. 1). In particular, the ground state of the well (which in one dimension exists as long as $V(x,t) < 0$ [15]) will turn before reaching the continuum threshold if $\mathcal{E} < 0$, "just touch" it if $\mathcal{E} = 0$, or disappear at $t = -\sqrt{\mathcal{E}}/v$, before reappearing again at $t = \sqrt{\mathcal{E}}/v$, if $\mathcal{E} > 0$. In all three cases, we are interested in the probabilities P_{mn}^{stay} defined in Eq. (5).

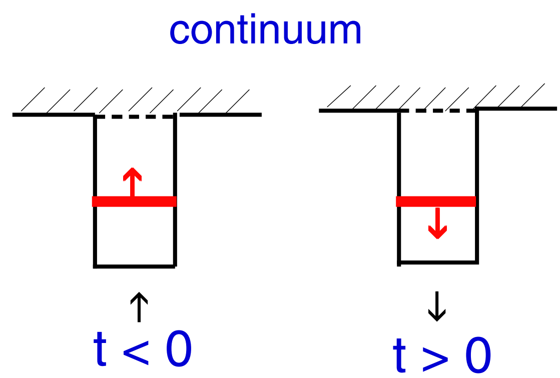

FIG. 1. (Color online) Schematic diagram showing the evolution of the potential well described by Eq. (6). At first the well becomes shallower, thus bringing its bound state [thick (red) horizontal line with arrow] closer to the continuum. Later the well deepens, bringing the state down and, possibly, bringing more bound states into the well. At $t = 0$, the bound state may still exist if $\mathcal{E} < 0$, may touch the continuum threshold if $\mathcal{E} = 0$, or may disappear for a while if $E > 0$.

III. STURMIAN EXPANSION OF THE TIME-DEPENDENT STATE

With the help of the Fourier transform,

$$\Psi(x,t) = \int d\omega \exp(-i\omega t)\Psi(x,\omega), \tag{7}$$

we rewrite Eq. (2) as

$$\omega\Psi(x,\omega) = -\partial_x^2\Psi/2\mu - W(x)\sum_{k=0}^{K}(-i)^k V^{(k)}\partial_\omega^k\Psi \tag{8}$$

and look for a suitable basis in which to expand $\Psi(x,\omega)$. Using the set of the positive-energy scattering states describing particles incident on $V(x,t)$ from left and right is one option, yet there is a more convenient one. Particles ejected from the well should be described by outgoing waves on both sides of the potential. Sturmian basis sets with the desired properties are well known in the literature [19]. They are obtained by imposing outgoing boundary conditions, fixing the value of ω in Eq. (8), and searching for particular shapes of $V_n(x,t) = \rho_n W(x)$, $n = 1,2,\ldots$, such that the stationary SE

$$-\partial_x^2 S_n/2\mu + \rho_n W(x)S_n = \omega S_n, \quad n = 0,1,2,\ldots, \tag{9}$$

has a solution $S_n(x,\omega)$ which satisfies the boundary conditions

$$S_n(x,\omega) \sim \exp(\pm i\sqrt{2\mu\omega}x), \quad x \to \pm\infty. \tag{10}$$

The Sturmian eigenfunctions S_n (also known as Sturmians) differ for positive and negative ω's. As seen from Eq. (10), for $\omega < 0$, all $S_n(x)$ exponentially decay on both sides of the well, $S_n(x) \sim \exp(-\sqrt{2\mu|\omega|}|x|)$ for $|x| \to \infty$, so that $\rho_n W(x)$ has a bound state at the chosen energy ω [21]. For $\omega > 0$, the Sturmian contains outgoing traveling waves, $S_n(x,\omega) \sim \exp(\pm i\sqrt{2\mu\omega}|x|)$, as $x \to \pm\infty$. This can only be the case if $\rho_n W(x)$ is a complex-valued emitting potential, which, in turn, requires $\text{Im}\rho_n > 0$ for $\omega > 0$. In general, as ω changes from $-\infty$ to $+\infty$, a chosen $\rho_n(\omega)$ traces a continuous trajectory in the complex ρ plane.

From Eq. (9) follows an orthogonality relation,

$$(S_m(\omega)|S_n(\omega)) \equiv \int S_m(x,\omega)W(x)S_m(x,\omega)dx$$
$$= \delta_{mn} \times (S_n(\omega)|S_n(\omega)), \tag{11}$$

where δ_{mn} is the Kroneker delta. The Sturmians are also known to form complete sets for both $\omega < 0$ and $\omega > 0$ (we refer the reader to Ref. [18] for a detailed discussion). Thus, to construct a physical solution $\Psi(x,t)$ describing particles which escape from the trap, we expand $\Psi(x,\omega)$ in (8) in the basis of S_n,

$$\Psi(x,\omega) = \sum_n B_n(\omega)S_n(x,\omega), \tag{12}$$

where the coefficients $B_n(\omega)$ are to be determined. Inserting (12) into Eq. (8), after adding and subtracting $\sum_n \rho_n W B_n S_n$, we have

$$\sum_n \left\{ \sum_k (-i)^k V^{(k)} W(x)\partial_\omega^k [B_n(\omega)S_n(x,\omega)] + \rho_n W(x)B_n(\omega)S_n(x,\omega) \right\} = 0. \tag{13}$$

In our quadratic case, (6), multiplication of Eq. (13) by $S_m(x,\omega)$ and integration over x yield the following set of equations for $B_n(\omega)$,

$$M_{mm}^{(0)}[v^2 B_m'' + (\mathcal{E} - \rho_m)B_m] - v^2 \sum_n \left(2M_{mn}^{(1)} B_n' + M_{mn}^{(2)} B_n\right) = 0, \tag{14}$$

where a prime denotes differentiation with respect to ω, and

$$M_{mn}^{(j)} \equiv \int S_m(x,\omega)W(x)\partial_\omega^j S_n(x,\omega)dx$$
$$\equiv (S_m(\omega)|S_n^{(j)}(\omega)). \tag{15}$$

Equations (14) and (15) are the main achievement of the Sturmian approach: the problem of solving a partial differential equation, (2), is reduced to one of solving a system of second-order ordinary differential equations. With only a few terms usually needed in Eq. (14), the Sturmian approach offers a significant computational advantage in the case of many dimensions [17–20]. In the one-dimensional case considered here, it can offer further insight into the physics of scattering by time-dependent potentials and simplify calculations in certain limiting cases, as we demonstrate next.

IV. QUADRATIC ZERO-RANGE MODEL: THE ADIABATIC LIMIT

We start with the simplest case of a zero-range potential,

$$W(x) = \delta(x), \tag{16}$$

which for $\mathcal{E} - v^2t^2 < 0$ supports a single adiabatic bound state [$\theta(x) = 1$ for $x \geqslant 0$ and 0 otherwise],

$$\phi_0(x,t) = [-2\mu E_0(t)]^{1/4}\left[\theta(x)\exp(i\sqrt{2\mu E_0(t)}x) + \theta(-x)\exp(-i\sqrt{2\mu E(t)}x)\right], \tag{17}$$

with energy

$$E_0(t) = -\mu(\mathcal{E} - v^2t^2)^2/2. \tag{18}$$

There is only one Sturmian [16,20],

$$S_0(x,\omega) = [\theta(x)\exp(i\sqrt{2\mu\omega}x) + \theta(-x)\exp(-i\sqrt{2\mu\omega}x)], \tag{19}$$

and the corresponding Sturmian eigenvalue, given by

$$\rho_0(\omega) = i\sqrt{2\omega/\mu}, \tag{20}$$

is single-valued on a two-sheet Riemann surface $\mathcal{R}$ of $\sqrt{\omega}$, cut along the positive semiaxis. With no other Sturmians present, and $M_{00}^{(2)} = 0$ since $S(0,\omega) = 1$, taking the complex conjugate of Eq. (14) [22] yields

$$B_0^{*\prime\prime} + v^{-2}q^2 B_0^* = 0, \quad q(\omega) \equiv \sqrt{\mathcal{E} - \rho_0^*(\omega)}. \tag{21}$$

Equation (21) must be integrated along the contour running along the real ω axis above the cut of the first sheet of $\mathcal{R}$, where $S_0(x,\omega)$ satisfies the required outgoing-decaying wave boundary conditions, (10).

Equation (21), which is exact, can now be read in a completely different manner. It has the form of a stationary SE describing a "particle" of "mass" 1/2 with a "coordinate" ω, of "energy" $\mathcal{E}$, scattered by a "potential" $\mathcal{W}(\omega) = \rho_0^*(\omega)$, with v playing the part of the "Planck constant" $\hbar$ [23]. [We always use quotation marks when we refer to the fictitious "particle" in Eq. (21), in order to distinguish it from the real particle described by the SE, (2)]. We note that the "potential" $\mathcal{W}$, shown in Fig. 2, has a valley (Re$\mathcal{W} < 0$, Im$\mathcal{W} = 0$) for $\omega < 0$ and becomes purely absorbing (Re$\mathcal{W} = 0$, Im$\mathcal{W} < 0$) for $\omega > 0$.

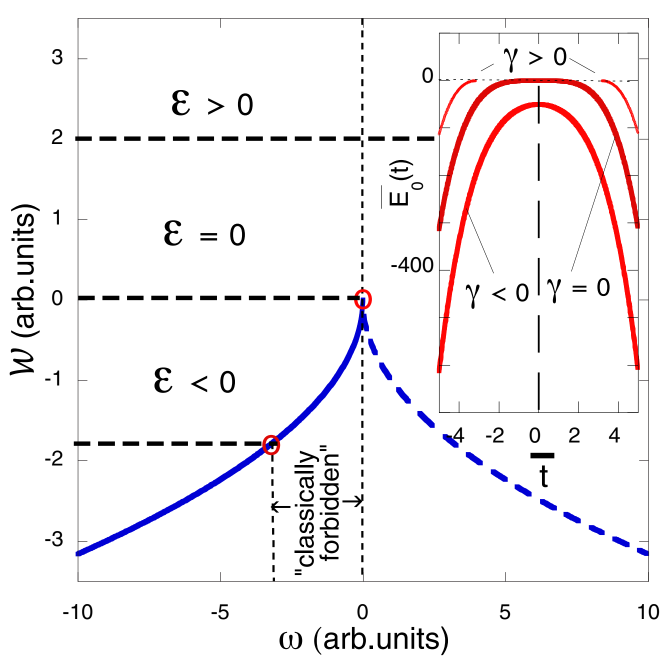

FIG. 2. (Color online) Schematic diagram of the zero-range model. A "particle" with "energy" $\mathcal{E}$ is scattered by a complex-valued "potential," $\mathcal{W}$, whose real and imaginary parts are shown by the solid and dashed lines, respectively. Also indicated is the "classically forbidden region," separating a "particle" with $\mathcal{E} < 0$ from the absorption region, $\omega > 0$. Inset: The energy of the bound state given by (18), $\overline{E}_0(t) = \mu^{-1/5}v^{-4/5}E_0(t)$, as a function of $\overline{t} = \mu^{1/5}v^{4/5}t$.

Properties of equations of the type of (21) are well known (see, e.g., [15]). As $\omega \to -\infty$, $q(\omega) \to \infty$, while $\mathcal{W}(\omega)$ becomes flatter, $\mathcal{W}'(\omega) \sim 1/\sqrt{|\omega|} \to 0$, so that $B(\omega)$ can be expressed in semiclassical form [15], in terms of incoming (+) and outgoing (–) "waves,"

$$B_0^*(\omega) \approx \frac{A^+}{\sqrt{q(\omega)}} \exp\left[\frac{i}{v}\int^{\omega} q(\omega')d\omega'\right] + \frac{A^-}{\sqrt{q(\omega)}} \exp\left[-\frac{i}{v}\int^{\omega} q(\omega')d\omega'\right], \quad \omega \to -\infty, \tag{22}$$

where $A_\pm$ are unknown constants to be determined. We do not expect the particle to acquire a very high energy and must, therefore, require that $B(\omega) \to 0$ as $\omega \to \infty$. Thus, taking the principal branch of the square root in Eq. (21), we have

$$B^*(\omega) \sim \frac{1}{\sqrt{q(\omega)}} \exp\left[-\frac{1}{v}\int^{\omega} |q(\omega')|d\omega'\right] \to 0, \quad \omega \to \infty. \tag{23}$$

Finally, inserting (12) and (22) into Eq. (7) we note that as $t \to \pm\infty$ the integral over ω may be evaluated by the stationary-phase method [25], and as $t \to -\infty$ we have (details are given in Appendix A)

$$\Psi(x,t) \approx 2v\sqrt{\pi i}A^+\phi(x,t)\exp\left[-i\int^t E_0(t')dt'\right]. \tag{24}$$

This describes a particle trapped in the ascending bound state, which approaches the continuum threshold from below. Similarly, for $t \to \infty$ we have

$$\Psi(x,t) \approx 2v\sqrt{-\pi i}A^-\phi(x,t)\exp\left[-i\int^t E_0(t')dt'\right] + \delta\Psi(x,t), \tag{25}$$

where the first term describes a particle trapped in the descending bound state, moving away from the continuum threshold. For the probability of completing the passage and remaining in the bound state, we therefore have

$$P_{00}^{\text{stay}} = \frac{|A_-|^2}{|A_+|^2}, \tag{26}$$

which is $\leqslant 1$, as guaranteed by the absorbing nature of the "potential" for $\omega > 0$. (More information on absorbing boundary conditions for the SE can be found, e.g., in [26], and references therein).

Reduction of the original time-dependent problem to one of determining the reflection coefficient of a complex-valued barrier allows us to prove the existence of the adiabatic limit in the case where the bound state turns without touching the continuum $\mathcal{E} < 0$. Now absorption represents the loss of the particle to the continuum, and to be absorbed, the "particle" must first cross the "classically forbidden region" (see Fig. 2), impenetrable in the "classical limit" $v \to 0$. This is the *adiabatic theorem*. The behavior at $\mathcal{E} \geqslant 0$ requires somewhat more attention, and we consider it next.

V. A ZERO-RANGE WELL: JUST TOUCHING THE CONTINUUM

With $\mathcal{E} = 0$, we have $E_0(t = 0) = 0$, so the bound state of a zero-range well approaches the continuum threshold and touches it at the moment it turns to begin the downward leg of its journey. In this special case the equation for B_0,

$$B_0'' + b\sqrt{\omega}B_0 = 0, \quad b = \sqrt{2/\mu}\exp(3\pi i/2)/v^2, \tag{27}$$

can be solved analytically in terms of the Bessel functions [27]. The solution which vanishes as $\omega \to \infty$ is given by

$$B(\omega) = \sqrt{\omega}H_{2/5}^{(1)}(z), \quad z \equiv \frac{2^{9/4}}{5v}e^{3\pi i/4}\omega^{5/4}, \tag{28}$$

where $H_\nu^{(j)}(z)$, $j = 1,2$, is the Hankel function of the jth kind [28]. As $\omega \to \infty$, we have (omitting inessential phase factors)

$$B(\omega) \sim \omega^{-1/8}\exp[-(1+i)K\omega^{5/4}]_{\omega\to\infty} \to 0, \tag{29}$$

where $K \equiv 2^{7/4}/5\mu^{1/4} > 0$. Equation (29) is readily recognized as a special case of Eq. (23), with $q(\omega) = (2\omega/\mu)^{1/4}\exp(-i\pi/4)$. To find the asymptotic form of $B(\omega)$ for $\omega \to -\infty$, we use the formula connecting the values of $H_{2/5}^{(1)}(z)$ on the ray $z' = \rho\exp(3\pi i/4)$ with those along $z = z'\exp(i\pi) = \rho\exp(7\pi i/4)$ (see [28], Sec. 3.62):

$$H_{2/5}^{(1)}(z') = 2\cos(2\pi/5)H_{2/5}^{(1)}(z) + \exp(-2\pi i/5)H_{2/5}^{(2)}(z). \tag{30}$$

Recalling that $H_\nu^{(1,2)}(z) \sim (2/\pi z)^{1/2}\exp[\pm i(z - \nu\pi/2 - \pi/2)]$ [28], and taking the complex conjugate of Eq. (30), we identify $H_{2/5}^{(2)}(z)$ with the incoming wave in Eq. (22), which gives

$$P_{00}^{\text{stay}}(v) = 4\cos^2(2\pi/5) \approx 0.38197. \tag{31}$$

Thus, for a narrow well such that its bound state just touches the continuum at $t = 0$, the probability of remaining in the well is independent of the rate of change of the potential. There is a perfect balance: a rapidly changing well is more likely to eject the particle into the continuum, yet the time the bound state spends near the threshold is short. If the well changes slowly, this time is longer, yet the particle is ejected less efficiently. As a result, there is no adiabatic limit as $v \to 0$, and the value of P_{00}^{stay} is always given by Eq. (31). Below we show that Eq. (31) has a more general meaning also, beyond the zero-range model considered in this section.

VI. A ZERO-RANGE WELL: THE GENERAL CASE

No analytic solution of (27) is known (at least to us) for $\mathcal{E} \neq 0$, so the equation must be solved numerically. We note first that, for a narrow well, (16), P_{00}^{stay} is determined by a single dimensionless parameter,

$$\gamma \equiv \frac{\mathcal{E}\mu^{2/5}}{v^{2/5}}. \tag{32}$$

Indeed, in the scaled variables $\tau = \mu^{1/5}v^{4/5}t$ and $y = \mu^{3/5}v^{2/5}x$, the SE, (2), reads $i\partial_\tau\Psi(y,\tau) = -\partial_y^2\Psi/2 + (\gamma - \tau^2)\delta(y)\Psi$, and Eq. (27) only needs to be solved for $v = 1$ and various values of $\mathcal{E} = \gamma$. The dependence of $P_{00}^{\text{stay}}(\gamma)$ on γ is shown in Fig. 3. The probability tends to 1 for $\gamma \to -\infty$, where the "absorbing potential" in Fig. 2 is

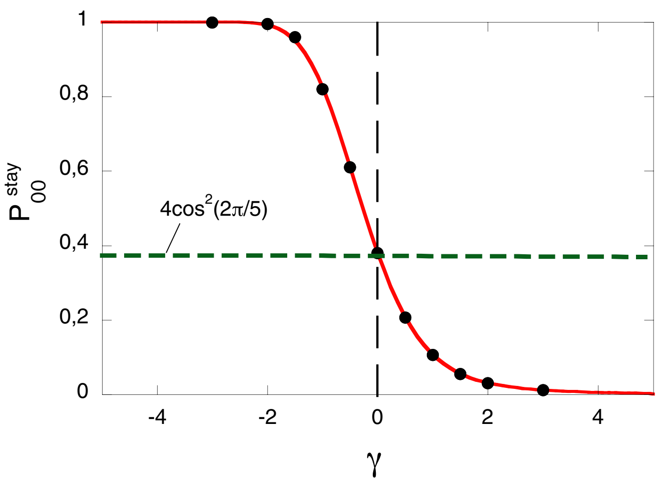

FIG. 3. (Color online) Probability $P_{00}^{\rm stay}$ vs γ for the quadratic zero-range model, (16), obtained by integrating Eq. (21) [solid (red) curve] and by solving numerically the original SE, (2) (filled circles).

separated by a broad "classically forbidden" region. At $\gamma = 0$ the curve passes through the value given by Eq. (31), $P^{\rm stay}(0) = 4\cos^2(2\pi/5)$, and tends to 0 as $\gamma \to \infty$, i.e., when the "particle" can penetrate deep into the "absorbing region," and nothing is reflected.

Using Fig. 3, it is easy to predict the behavior of the retention probability $P^{\rm stay}$ as a function of v, for a given $\mathcal{E}$. For $\mathcal{E} < 0$ and $v \ll \mu|\mathcal{E}|^{5/2}$ the passage will be adiabatic, with almost none of the particles lost. For $\mathcal{E} > 0$ and $v \ll \mu|\mathcal{E}|_0^{5/2}$, the bound state will disappear for a long time (see inset in Fig. 2), and none of the particles will be recovered when it finally reappears. With $v \to \infty$, γ will vanish for any choice of $\mathcal{E}$, and we have

$$\lim_{v\to\infty} P_{00}^{\rm stay}(\mathcal{E},v) = 4\cos^2(2\pi/5), \tag{33}$$

so that a rapidly changing zero-range well will retain the particle in about 38% of all cases, regardless of the value of $\mathcal{E}$. The dependence of $P_{00}^{\rm stay}(\mathcal{E},v)$ on v for different values of $\mathcal{E}$ is shown in Fig. 4.

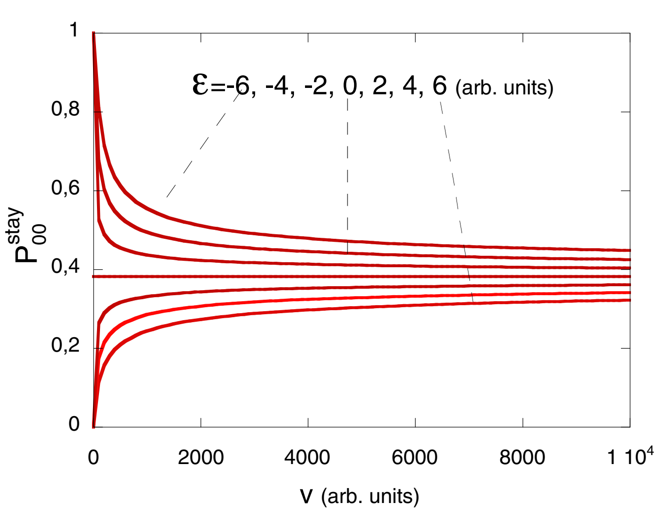

FIG. 4. (Color online) Probability $P_{00}^{\rm stay}$ vs v for the quadratic zero-range model, (16), for different values of $\mathcal{E}$.

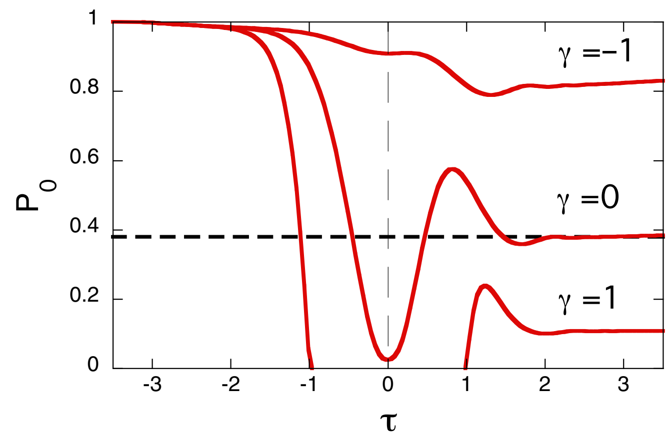

FIG. 5. (Color online) The population of the moving bound state, $P_0(t) = |\langle\phi_0(t)|\Psi(t)\rangle|^2$, vs $\tau = \mu^{1/5}v^{4/5}t$ for three values of $\gamma = \mathcal{E}\mu^{2/5}v^{-2/5}$. For $\gamma = 1$ the bound state disappears at $\tau = -1$ and reappears again at $\tau = 1$.

Finally, in order to study the evolution of the population $P_0(t)$ of the moving bound state, we solved numerically the original SE, (2). The results shown in Fig. 5 demonstrate that $P_0(t) \equiv |\langle\phi_0(t)|\Psi(t)\rangle|^2$ undergoes oscillations before reaching the asymptotic value $P_0(t) = P_{00}^{\rm stay}$, when the bound state is well removed from the continuum.

VII. A RECTANGULAR WELL: THE ADIABATIC LIMIT

The more realistic case of a rectangular well of width $2a$,

$$W(x) = [\theta(x+a)\theta(a-x)]/2a, \tag{34}$$

is somewhat more involved. There are two types of Sturmians, symmetric and antisymmetric about the origin, $S_n(x,\omega) = S_n(-x,\omega)$ and $T_n(x,\omega) = -T_n(-x,\omega)$. For $-a \leqslant x \leqslant a$, these are given by

$$S_n(x,\omega) = \cos(p_n x)/[1+\sin(2p_n a)/2p_n]^{1/2}, \quad n = 0,2,4,\ldots, \tag{35}$$

and

$$T_n(x,\omega) = \sin(p_n x)/[1-\sin(2p_n a)/2p_n]^{1/2}, \quad n = 1,3,5\ldots, \tag{36}$$

so that $(S_n|S_n) = (T_n|T_n) = 1$. Since the matrix elements in Eq. (14) couple only Sturmians of the same parity, $(S_m(\omega)|T_n^{(j)}(\omega)) = (T_m(\omega)|S_n^{(j)}(\omega)) = 0$, we may limit our analysis to the case where a particle is prepared initially in a bound state symmetric about the origin. The corresponding Sturmian eigenvalues ρ_n, $n = 0, 2, 4, \ldots$, are then found by solving a transcendental equation,

$$\sin(p_n a)/\cos(p_n a) + ik/p_n = 0, \tag{37}$$

where

$$p_n(\omega) = \{2\mu[\omega - \rho_n(\omega)]\}^{1/2} \quad \text{and} \quad k(\omega) = (2\mu\omega)^{1/2}. \tag{38}$$

Thus, $\rho_n(\omega)$, is the magnitude of the rectangular potential, real or complex, such that at a given energy ω, there is

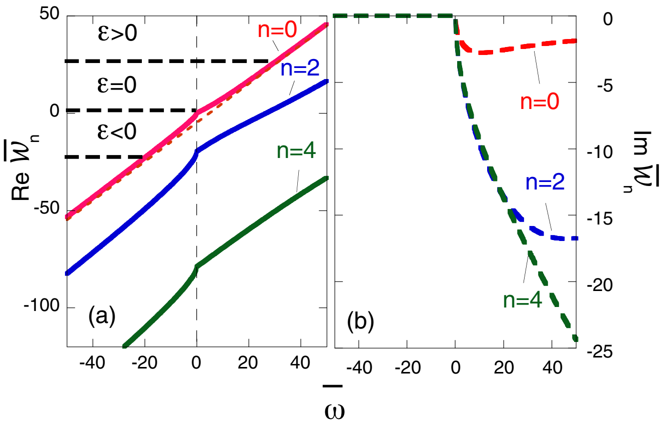

FIG. 6. (Color online) (a) Real and (b) imaginary parts of the "channel potentials" $\overline{\mathcal{W}}_n = \mu a \mathcal{W}_n$ vs $\overline{\omega} = \mu a^2\omega$ for $n = 0$, 1, 2. In (a), also shown by the dashed line is the large-ω asymptote of Re$\mathcal{W}_0$, $\omega a - \pi^2/2\mu a$.

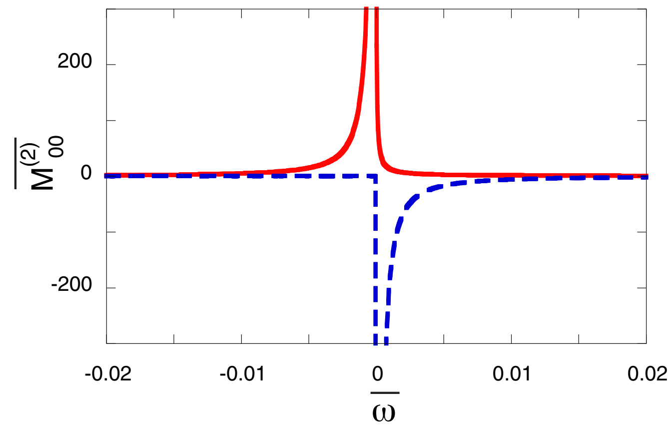

FIG. 7. (Color online) Real (solid curves) and imaginary (dashed curves) parts of the correction term $\overline{M^{(2)}_{00}} = \mu a M^{(2)}_{00}$ vs $\overline{\omega} = \mu a^2\omega$.

a symmetric solution $S_n(x)$ of the SE, (9), satisfying the boundary conditions, (10).

The interpretation of equations for $B^*_n(\omega)$ is similar to that given in Sec. IV. One may think of a fictitious "particle" with "energy" $\mathcal{E}$ which can move on several complex-valued "potential surfaces" $\mathcal{W}_n(\omega) = \rho^*_n(\omega)$. On each surface, absorption, possible at $\omega > 0$, accounts for the loss of the real particle to the continuum. There is also the possibility of hopping between the "surfaces," facilitated by matrix elements $M^{(1)}_{mn}(\omega)$ and $M^{(2)}_{mn}(\omega)$. If a particle is prepared in the mth state of the deep well, we must look for a solution of this "coupled-channels problem" containing, as $\omega \to -\infty$, an incoming wave on the mth "potential surface" and, possibly, "outgoing waves" in all other "channels,"

$$B^*_n(\omega) \sim \delta_{mn}\frac{A^+_m}{\sqrt{q_m}}\exp\left[\frac{i}{v}\int^{\omega} q_m(\omega')d\omega'\right] + \frac{A^-_n}{\sqrt{q_n}}\exp\left[-\frac{i}{v}\int^{\omega} q_n(\omega')d\omega'\right], \quad \omega \to -\infty, \tag{39}$$

where $m,n = 0,2,4\ldots$. The probabilities of a particle's starting in the mth and ending up in the nth adiabatic bound states are given by

$$P^{\rm stay}_{mn} = \frac{|A^-_n|^2}{|A^+_m|^2}, \quad m,n = 0,2,4,\ldots. \tag{40}$$

The "potentials" $\mathcal{W}_n(\omega)$ are shown in Fig. 6 for $m = 0,2,4$. We have Im$\mathcal{W}_n(\pm) \equiv 0$ for $\omega < 0$, where Sturmians are just bound states of a real potential well. We also note that

$$\lim_{\omega\to\pm\infty} {\rm Re}\mathcal{W}_n(\omega) = \omega a - (2n+1)^2\pi^2/2\mu a \tag{41}$$

and

$$\lim_{\omega\to\infty} {\rm Im}\mathcal{W}_n(\omega) = 0. \tag{42}$$

This is because for a large negative ω, the Sturmians tend to the eigenstates of a potential box with infinite walls at $x = \pm a$. Since the energy of the state is ω, ρ_n is found by subtracting from ω the energy of the nth state, as measured from the floor of the well. In the opposite limit, $\omega \to \infty$, the particle becomes bound at the top of an infinitely high rectangular barrier. These bound states, quantized between the sharp potential drops at $x = \pm a$, are essentially the same as those quantized between the walls of an infinite potential box [29]. Since the Sturmians cease to depend on ω as $\omega \to \pm\infty$,

$$S_n(x,\omega) \sim \theta(x+a)\theta(a-x)\cos[(2n+1)\pi x/2a], \tag{43}$$

the matrix elements, coupling the "potential surfaces,", vanish in the same limit,

$$M^{(1,2)}_{mn}(\omega) \to 0, \quad \omega \to \pm\infty. \tag{44}$$

Both $M^{(1)}_{mn}$ and $M^{(2)}_{mn}$ are singular at the threshold $\omega = 0$, as explained in Appendix B. In particular, for $M^{(2)}_{00}$, which is required in the next section, we find $M^{(2)}_{00}(\omega) \sim \omega^{-1.5}$ (see Fig. 7).

We can now formulate the adiabatic limit for a particle prepared in the ground state of a rectangular well, $m = 0$, at $t \to -\infty$, provided the state turns before reaching the continuum threshold, $\mathcal{E} < 0$. As in the case of the zero-range potential, the "absorbing region" is separated by a "classically forbidden region" in Fig. 6 and becomes inaccessible for a "particle" incident on the $n = 0$ "potential surface" as $v \to 0$. There is, however, the possibility of accessing the "absorbing potential" in Fig. 6 by hopping to a different "potential surface." But as $v \to \infty$ the hopping also becomes improbable, since the solutions on different "surfaces" become highly oscillatory, and the integrals involving $M^{(1,2)}_{0n}(\omega)$ vanish. We, therefore, have the adiabatic limit

$$P^{\rm stay}_{0n}(\mathcal{E} < 0, v \to 0) \to \delta_{0n}. \tag{45}$$

This result is easily extended to other initial states, $m \neq 0$. The behavior at other values of $\mathcal{E}$ and v requires more attention, and we consider it next.

VIII. A RECTANGULAR WELL: THE SINGLE-STURMIAN APPROXIMATION

The above discussion suggests that if the trapping potential changes sufficiently slowly, one can largely neglect scattering into other bound states of the well, thus leaving a few Eq. (14)

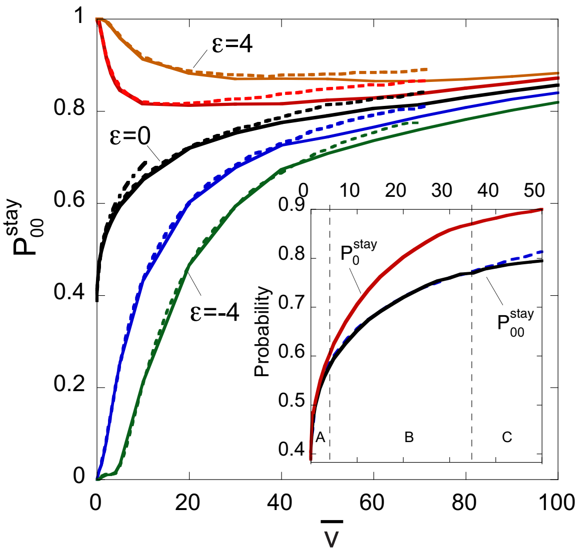

FIG. 8. (Color online) Probability of remaining in the ground state of a rectangular well, P_{00}^{stay}, vs $\overline{v} = 8\mu^{3/2}a^3 v$ for $\overline{\mathcal{E}} = -4$, -2, 0, 2, 4 (solid curves). Also shown are the single-Sturmian approximations to these probabilities obtained with (dashed curves) and without (dot-dashed curve) the last term in Eq. (46). Inset: Total probability P_0^{stay} [thick solid (red) curve], exact P_{00}^{stay} (solid black curve), and single-Sturmian approximation to P_{00}^{stay} [dashed (blue) curve]. Dashed vertical lines indicate the three regimes described in Sec. VIII.

or, indeed, just one Eq. (14). For a particle arriving in the adiabatic ground state, $m = 0$, we, therefore, write

$$B_0^{*\prime\prime} + \left[v^{-2}(\mathcal{E} - \rho_0^*) + \left(S_0\middle|\partial_\omega^2 S_0\right)^*\right]B_0^* = 0, \tag{46}$$

where we have retained the diagonal correction term $M_{00}^{(2)}(\omega)$. With no analytical solution available for Eq. (46), we have to solve it numerically.

In the dimensionless variables $\tau = 4ma^2 t$, $y = x/2a$, $[\overline{\mathcal{E}} = 4\mu a^2\mathcal{E}$, and $\overline{v} = 8\mu^{3/2}a^3 v$, the SE, (2), reads $i\partial_\tau\Psi(y,\tau) = -\partial_y^2\Psi/2 + [\overline{\mathcal{E}} - \overline{v}^2\tau^2)]\theta(y+1/2)\theta(1/2-y)\Psi$, and we must solve Eq. (46) for a particle of unit mass in a well of unit length, replacing ω with $\mu a^2\omega$. The results for P_{00}^{stay} are shown in Fig. 8 together with the exact curves, obtained by solving numerically the original SE, (2).

The exact results are worth a brief discussion. For the ground state just touching the continuum threshold, $\overline{\mathcal{E}} = 0$, the P_{00}^{stay} tends to the constant value in Eq. (31),

$$P_{00}^{\text{stay}}(\overline{\mathcal{E}} = 0, \overline{v} \to 0) \to 4\cos^2(2\pi/5). \tag{47}$$

This can be understood by scaling the variables in Eq. (2) in a different way, so as to put to unity the particle's mass μ as well as v, i.e., $\tau = m^{1/5}v^{4/4}t$, i.e., $y = \mu^{3/5}v^{2/5}x$. With this we also have $W(y) = [\theta(y + \mu^{3/5}v^{2/5}a)\theta(\mu^{3/5}v^{2/5}a - y)]/2\mu^{3/5}v^{2/5}a$. As $v \to 0$, the width of $W(y)$ tends to 0, and we recover the zero-range result, (47), which holds universally for all values of v and, in particular, for $v = 1$.

For a rapidly changing rectangular trap, $\overline{v} \to \infty$, the particle always returns to the well, regardless of whether the adiabatic state turns before touching the continuum, just touches it, or even disappears for a while. A different type of scaling can be used to explain why. Putting to unity the well's width as well as v, we have a particle of mass $\overline{\mu} = 4a^2v^{2/3}\mu$ and a new parameter, $\overline{\mathcal{E}} = \mathcal{E}/v^{2/3}$. As $v \to \infty$, we have a picture of a very heavy particle, $\overline{\mu} \to \infty$, brought to the continuum threshold, $\overline{\mathcal{E}} \to 0$, and then down again. The massive particle has no chance to escape, and we have

$$P_{00}^{\text{stay}}(\overline{\mathcal{E}}, \overline{v} \to \infty) \to 1, \tag{48}$$

which holds for all finite values of $\overline{\mathcal{E}}$.

Finally, if a bound state disappears, the particle's state is a wave packet of continuous states, which spends a duration of $2\sqrt{\mathcal{E}}/v$ spreading away from the region. For $v \to 0$ the time of spreading is very long, so that little is recaptured after the bound state reappears at $t = \sqrt{\mathcal{E}}/v$. Thus we have

$$P_{00}^{\text{stay}}(\overline{\mathcal{E}} > 0, \overline{v} \to 0) \to 0. \tag{49}$$

The single-Sturmian approximation for P_{00}^{stay}, obtained by solving Eq. (46), is in good agreement with the exact result for $\overline{v} \lesssim 40$. Comparing the two curves with the total probability of staying in the well, $P_0^{\text{stay}} = \sum_n P_{0n}^{\text{stay}}$, shown in the inset in Fig. 8 helps identify three approximate regimes.

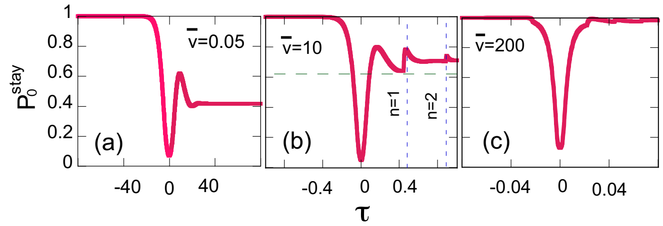

FIG. 9. (Color online) Rectangular barrier. (a) P_0^{stay} vs $\tau = 4\mu a^2 t$ for $\overline{v} = 0.05$. (b) Same as (a), but for $\overline{v} = 10$. Dashed vertical lines indicate the moments when the first and the second excited states enter the well. (c) Same as (a), but for $\overline{v} = 200$.

A. Slow passage

For $\overline{v} \lesssim 5$, we have $P_0^{\text{stay}} \approx P_{00}^{\text{stay}}$. The loss and recapture of particles are determined by interaction of a single bound state with the continuum. There is no scattering into other bound states. Mathematically, the problem reduces to solving a single equation, (46) [see Fig. 9(a)].

B. Intermediate passage

For $5 \lesssim \overline{v} \lesssim 80$, we have $P_0^{\text{stay}} > P_{00}^{\text{stay}}$, $(P_0^{\text{stay}} - P_{00}^{\text{stay}})/P^{\text{stay}} \ll 1$, where P_{00}^{stay} is correctly described by Eq. (46). This suggests that a downward-bound initial state recaptures some of the particles, and later each new bound state which enters the deepening well scoops some more [see Fig. 9(b)]. This regime can be described by solving Eq. (14) iteratively, using the solution of (46) as an initial approximation.

C. Rapid passage

For $80 \lesssim \overline{v}$ we find notable discrepancies between the single-Sturmian approximation for P_{00}^{stay} and the exact result. This indicates that the loss to continuum is accompanied also by transitions between different bound states. Mathematically, this requires solution of the full coupled-channels problem, (14) [see Fig. 9(c)]. We note that in the case of several spatial dimensions reduction of the original problem, (2), to that of solving a system of ordinary differential equations may be a significant simplification.

IX. UNIVERSALITY OF THE 38% RULE IN THE $v \to 0$ LIMIT

We have shown that in the two cases considered above, there is no conventional adiabatic limit for a ground state just touching the continuum threshold. Rather, as $v \to 0$, the probability of remaining in the state is given by Eq. (31) and equals approximately 38%. It easy to show that, for a quadratic evolution, (6), this result holds true in one dimension for a finite-width potential of an arbitrary form. Indeed, scaling the time and coordinate so as to put to unity v and the particle's mass μ, while maintaining the normalization $\int W(x)dx = 1$,

$$\tau = \mu^{1/5}v^{4/5}\tau, \quad y = \mu^{2/5}v^{2/5}x, \tag{50}$$

converts the SE (2) ($V^{(0)} = 0$) into

$$i\partial_\tau \Psi(x,t) = -\partial_y^2\Psi/2 + \tau^2\overline{W}(y)\Psi, \tag{51}$$

where $\overline{W}(y) \equiv \mu^{-3/5}v^{-2/5}W(\mu^{-3/5}v^{-2/5}y)$. As $v \to 0$, we have $\overline{W}(y) \to \delta(y)$ for any choice of $W(x)$, so that P_{00}^{stay} is given by Eq. (31). To illustrate this, we plotted the results for a rectangular well, (34), and a cutoff parabolic potential,

$$W(x) = 1.5[\theta(x+a)\theta(a-x)]x^2/a^3, \tag{52}$$

in Fig. 10(a).

The case where the mth excited state of the well touches the continuum requires more attention. Let the evolution of the potential be such that at $t = 0$, in the potential $-V^{(0)}W(x)$, we have $E_m = 0$. Returning to Eq. (14) we note that as $v \to 0$, the last sum in it may be neglected. Also, in this limit absorption of the "particle" occurs in a small vicinity of $\omega = 0$. Thus, if we can demonstrate that, for $\omega \approx 0$, $B_m(\omega)$ satisfies Eq. (27), obtained earlier for a zero-range well, we have also proven that $P_{mm}^{\text{stay}}(v \to 0) = 4\cos^2(2\pi/5)$, for all m's and all potential shapes.

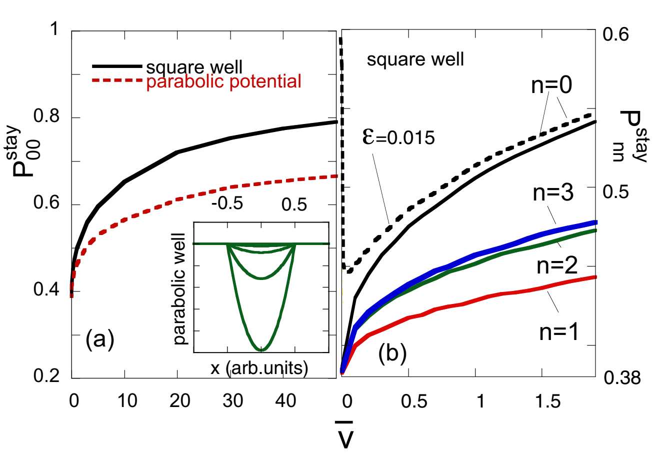

FIG. 10. (Color online) (a) Probabilities of remaining in the ground state of the square [dashed (red) curve] and parabolic (solid black curve) wells, P_{00}^{stay} for $\mathcal{E} = 0$, vs $\overline{v} = 8\mu^{3/2}a^3v$. Inset: Different shapes of the parabolic well, (52). (b) Same as (a), but for the first four states of a rectangular well touching the continuum threshold. The dashed line shows P_{00}^{stay} for $\mathcal{E} = -0.015$.

To show that this is the case, we use the standard approach, commonly used to describe potential scattering at low energies [24]. To this end, we consider a potential, $\rho W(x)$, whose mth bound state lies just below the threshold, construct a continuum state for a low positive energy, $\omega > 0$, and look for the condition under which the scattering amplitude diverges, $S(E,\rho) \to \infty$. Namely, our state will have the form $\exp(\pm ikx) + S(\omega,\rho)\exp(\mp ikx)$, $k = \sqrt{2\mu\omega}$, for $x \lessgtr a$. In the low-energy limit, $ka \ll 1$, the wavelength of the particle is large, and the well is characterized by a single parameter, the logarithmic derivative of the bound state's wave function at $x = \pm a$, which we denote $-\kappa$, so that $\phi_m(x,\rho) \sim \exp[-\kappa(\rho)x]$. We note that κ depends on the potential shape via ρ, but not on the energy ω, as long as ω is small. Matching the log-derivatives at $x = \pm a$, and using $ka \gg 1$ then yields

$$S(E,\rho) = \frac{ik - \kappa(\rho)}{ik + \kappa(\rho)}, \tag{53}$$

which diverges whenever $ik + \kappa(\rho) = 0$. The condition is usually used to obtain the pole in the complex ω plane, given a real value of ρ [24]. We, on the other hand, require the value of ρ, given a real value of ω, and need to make an additional assumption about how κ depends on ρ. The scattering length, defined as $\mathcal{L} = -1/\kappa$, is known to remain real, diverge, and change its sign as the shallow bound state moves toward the continuum threshold and, eventually, becomes a virtual state [24]. Thus, we assume κ to be a linear function of ρ,

$$\kappa(\rho) \approx C(\rho - \rho^0), \tag{54}$$

where $C > 0$ is a real constant and $E_m(\rho^0) = 0$. Solving the pole condition $ik + \kappa(\rho) = 0$ for ρ, we have

$$\rho_m(\omega) = i\sqrt{2\mu\omega}/C_m + \rho_m^0, \tag{55}$$

where we have recalled that our derivation is for a particle prepared in the mth state of the deep well and added the index m, where required. Inserting (55) into Eq. (14), neglecting all but one of them, and noting that $V^{(0)} = \rho_m^0$, for $\omega \approx 0$ we have

$$B_m{}'' + c\sqrt{\omega}B_m = 0, \quad c = -i\sqrt{2\mu}/C_m v^2. \tag{56}$$

The similarity between Eq. (27) and Eq. (57) in the region of interest allow us to conclude that for any state ϕ_m, $m = 0,1,2,\ldots$, touching the continuum threshold,

$$\lim_{v \to 0} P_{mn}^{\text{stay}} = 4\cos^2(2\pi/5)\delta_{mn} \simeq 0.3819 \times \delta_{mn}. \tag{57}$$

This general result is valid for any potential, provided the scattering length $\mathcal{L}$ has a simple pole when the bound state ϕ_m joins the continuum, $\mathcal{L}(\rho) \sim 1/(\rho - \rho^0)$, where $E_m(\rho^0) = 0$. This condition is fulfilled, for example, for a rectangular well, (34), with the results for various excited states, obtained by integrating Eq. (46), shown in Fig. 10(b).

To conclude this section, we note that any similarity between the rule, Eq. (57), and the celebrated 37% stopping rule of the statistical Secretary Problem [30] is fortuitous.

While the latter rule follows from simple combinatorial considerations and is, in fact an approximation to $1/e$, Eq. (57) is a consequence of the Stokes phenomenon experienced by the Hankel function in Eq. (28).

X. SUMMARY AND CONCLUSIONS

In summary, we have analyzed, in one dimension, the evolution of a particle prepared in a bound state of a trapping potential, whose magnitude has a simple maximum at $t = 0$, as described by Eq. (6). There are three possible scenarios for the state, which first approaches the continuum threshold and then moves away from it. It may (i) turn before reaching the continuum threshold, (ii) just touch it once, or (iii) cross the threshold and temporarily disappear. Whether the particle remains in the trap or is lost to the continuum depends on how fast the variation of the trapping potential is.

In the slow-passage limit, the particle always remains in its initial (mth) state, provided the state turns before reaching the threshold, in accordance with the adiabatic theorem. If the state touches the threshold, the probability of remaining in it P^{stay}_{mm} is approximately 38%. This result holds universally for all excited states and various potentials, under a very general assumption about the behavior of the scattering length, (54), and replaces the conventional adiabatic limit. It follows from the fact that in the slow-passage limit, scattering into other states can be neglected, and one recovers the picture of a single state interacting with a continuum. This is the situation which arises in the case of a zero-range potential, where we have an analytic solution, as described in Sec. V.

If the bound state disappears for a while, a particle ejected into the continuum has sufficient time to move away from the potential. Thus, there is 100% loss to the continuum, and nothing is recovered when the state reappears.

In the rapid-passage limit, the outcome depends on the choice of the potential. Thus, for a zero-range well, P^{stay}_{00} tends to the same 38% limit, regardless of whether the bound state turns, touches the threshold, or crosses it. This appears to be the consequence of a perfect balance between the time a bound state of a δ well spends near the threshold and the efficiency with which the particle is ejected. On the other hand, in the case of a rectangular potential, a rapidly evolving well always retains the particle in its original state, whichever the fate of the bound state.

The general case of a passage which is neither slow nor fast is conveniently studied in the Sturmian representation. Unless the potential changes very rapidly, it is sufficient to employ only one Sturmian state, and the task of solving the time-dependent SE, (2). reduces to that of evaluating the reflection coefficient of a complex-valued "potential," where absorption of a fictitious "particle" accounts for the loss of the real particle to the continuum. For larger values of v, several Sturmian states need to be taken into account, and the picture is that of a "particle" capable of moving on several absorbing "potential surfaces." In general, one can loosely identify three regimes. If the passage is sufficiently slow, the state ejects the particles on its way up and then recovers some of them on its way down. For faster variations, the original state recovers its share of the particles, while more particles are scooped by other states, which enter the well as its depth increases. At yet larger v's, the loss to the continuum is accompanied by scattering into other bound states, and one needs to solve a full coupled-channels problem, (14).

Verification of the above theory is within the capabilities of modern experimental techniques, e.g., of laser-based methods for containing cold atoms in quasi-one-dimensional traps. In particular, realization of a quasi-one-dimensional optical box trap was reported in [6]. The shape of the trapping potential can be manipulated externally, which allows one to use it, for example, for preparing the desired number of states by ejecting unwanted particles into the continuum [5,7–10]. In spite of the practical difficulty of assuring that the state just touches the threshold, this result should be amenable to experimental verification. Figure 10(b) shows P^{stay}_{00} for a state that turns shortly before reaching the continuum, $\mathcal{E} = -0.015$, then closely follows the $\mathcal{E} = 0$ curve before shooting up to its adiabatic limit $P^{\text{stay}}_{00} = 1$ for very small values of v. Thus, the condition $\mathcal{E}$ can be fulfilled approximately, provided that v is chosen to be not too small.

Among other advantages offered by the Sturmian technique is the simple interpretation of the adiabatic condition for a state which turns before reaching the threshold. In this case, in order to be absorbed the fictitious "particle" must first cross the classically forbidden region in Fig. 2. With v playing the role of "Planck's constant," this becomes improbable, if the passage is slow. The manner in which P^{stay}_{mm} tends to the adiabatic limit as $v \to 0$ can then be studied by evaluating the corresponding phase integrals. We consider this in our future work, as well as extending the analysis to several spatial dimensions, different temporal evolutions, and to the case of several identical bosons trapped in the same bound state.

ACKNOWLEDGMENTS

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APPENDIX A

For $t > 0$, the stationary-phase approximation to the integral, (7), evaluated along the contour specified in Sec. IV is given by

$$I(t) \equiv \int_\Gamma q(\omega)^{-1/2} S(\omega,x) \exp\left[-i\omega t + i\int_{\omega_0}^{\omega} q(\omega')d\omega'\right]d\omega$$
$$\approx [2\pi i/q(\omega_s)\Phi''(\omega_s)]^{1/2} S(\omega_s,x)\exp[i\Phi(\omega_s,t)], \quad \text{(A1)}$$

where $\Phi(\omega,t) \equiv -i\omega t + i\int_{\omega_0}^{\omega} q(\omega')d\omega'$, and $\omega_s < 0$ is defined by

$$q(\omega_s) = t. \quad \text{(A2)}$$

Given the time evolution of the magnitude of the δ potential, there are three quantities, each of which can be used as an independent variable. These are the time itself τ, the well's depth $V(\tau) = \mathcal{E}_0 - v^2\tau^2$, and the energy of the adiabatic bound state supported by the well $E(\tau) = -\mu V^2(\tau)/2$. It is readily seen that $q(\omega)$ in Eq. (21) gives the time τ, at which $E(\tau(\omega)) = \omega$,

$$q(\omega) = \tau(\omega) = [\mathcal{E} - i\sqrt{2\omega/\mu}]^{1/2}/v. \tag{A3}$$

Let the lower limit in the integral in the exponent in Eq. (A1) be $\omega_0 = -\mu\mathcal{E}^2/2$ if $\mathcal{E} \geqslant 0$ and 0 otherwise. This ensures that $q(\omega)$ is always real non-negative for $\omega < 0$. Changing variables, $\omega- \to \tau(\omega)$, and integrating by parts, we have

$$\int_{t(\omega_0)}^{t(\omega)} \tau d\omega/d\tau d\tau = \tau E(\tau)\Big|_{\tau=\tau(\omega_0)}^{\tau=\tau(\omega)} - \int_{\tau(\omega_0)}^{\tau(\omega)} E(\tau)d\tau. \tag{A4}$$

With $\tau(\omega_s) = t$ and either $\tau(\omega_0)$ or $E(\tau(\omega_0))$ vanishing, we have

$$\Phi(\omega_s) = -\int_{\omega_0}^{t} E(\tau)d\tau. \tag{A5}$$

For the second derivative of the phase, $\Phi''(\omega_s)$, and the pre-exponential factor, we obtain

$$\Phi''(\omega_s) = q'(\omega_s) = [dE(\tau)/d\tau|_{\tau=t}]^{-1} = -[2\mu v^2 t(\Omega_0 + v^2t^2)]^{-1} = -[2v^2t\sqrt{-2\mu E(t)}]^{-1}, \tag{A6}$$

$$g(\omega_s) \equiv S(x,\omega_s)/\sqrt{q(\omega_s)} = S(x,E(t))/\sqrt{t}. \tag{A7}$$

Inserting (A5), (A6), and (A7) into (A1) and using (17) yield the term which multiplies A_+ in Eq. (25). Equation (24) for $t < 0$ can now be obtained as the complex conjugate of Eq. (A3).

APPENDIX B

For a rectangular potential of unit width, $a = 1/2$, and a particle of unit mass, $\mu = 1$, we have

$$(S_m(\omega)|S_n(\omega')) = \frac{F((p_m + p_n)/2) + F((p_m - p_n)/2)}{[F(p_m)F(p_n)]^{1/2}} \equiv G(p_m,p_n), \tag{B1}$$

where $p_m(\omega) = [2(\omega - \rho_m(\omega)]^{1/2}$, $p_n(\omega') = [2(\omega - \rho_n(\omega')]^{1/2}$, and $F(x) \equiv \frac{\sin(x)}{x}$. Thus, the coupling matrix elements are given by

$$M_{mn}^{(1)} = \frac{\partial G(p_m,p_n)}{\partial p_n}\frac{dp_n}{d\omega'}\bigg|_{\omega'=\omega} \tag{B2}$$

and

$$M_{mn}^{(2)} = \frac{\partial G(p_m,p_n)}{\partial p_n}\frac{d^2p_n}{d\omega'^2} + \frac{\partial^2 G(p_m,p_n)}{\partial p_n^2}\left(\frac{dp_n}{d\omega'}\right)^2\bigg|_{\omega'=\omega}. \tag{B3}$$

The divergencies of $M_{mn}^{(1,2)}$ at $\omega = 0$ come from the derivatives of p_n, which has a branching singularity at $\omega' = 0$. It follows from Eq. (37) that, as $\omega' \to 0$, $p_0 \sim \omega'^{1/4}$ and $p_{n\neq 0} \sim \omega'^{1/2}$. Therefore, for $\omega \to 0$ we obtain $M_{mm}^{(1)} \equiv 0$ since $(S_m(\omega)|S_n(\omega)) = 1$,

$$M_{m0}^{(1)} \sim \omega^{-3/4} \quad \text{and} \quad M_{mn}^{(1)} \sim \omega^{-1/2} \quad \text{for} \quad m \neq 0,n. \tag{B4}$$

Similarly, since the first term in Eq. (B3) vanishes for $n = m$,

$$M_{00}^{(2)} \sim \omega^{-1.5} \quad \text{and} \quad M_{mm}^{(2)} \sim \omega^{-1} \quad \text{for} \quad m \neq 0. \tag{B5}$$

For $m \neq n$ the first term in Eq. (B3) dominates, which leads to

$$M_{m0}^{(2)} \sim \omega^{-1.75} \quad \text{and} \quad M_{mn}^{(2)} \sim \omega^{-1.5} \quad \text{for} \quad m \neq 0. \tag{B6}$$

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[21] For example, consider $\omega < 0$, and increase the (real) depth of the rectangular well. As the well gets deeper, new bound states will enter it from the continuum and then move downwards. Recording the well's depth each time the energy of a symmetric bound state coincides with ω will give a (real) Sturmian eigenvalue $\rho_n(\omega)$. Obviously, there are infinitely many such eigenvalues.

[22] Equations for $B^*(\omega)$ contain an absorbing "potential," responsible for the loss to the continuum. In the equations for $B(\omega)$, the "potential" is of the emitting kind, and their form is less appealing.

[23] This is by no means the only example where solving a time-dependent SE can be reduced to a stationary scattering problem. See, for example, Chapter 7 in [24].

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