Adiabaticity near a continuum threshold: An exactly solvable model

D. Sokolovski,[1,2] M. Pons,[3] and J. G. Muga[1,4]
[1]*Departmento de Química-Física, Universidad del País Vasco, UPV/EHU, Leioa, Spain*
[2]*IKERBASQUE, Basque Foundation for Science, E-48011 Bilbao, Spain*
[3]*Departmento de Física Aplicada I, EUITMOP, Universidad del País Vasco, UPV-EHU, Bilbao, Spain*
[4]*Department of Physics, Shanghai University, 200444 Shanghai, China*
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We consider a potential well whose shape changes with time, so that a bound state is brought closer to the edge of the continuum. We then ask the following: how slow should the evolution be for the adiabatic approximation to hold? We answer the question by considering, in a Sturmian representation, linear evolution of a δ-function potential well. The general applicability and accuracy of the obtained adiabatic criterion is discussed.

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I. INTRODUCTION

Recently, there has been a spectacular progress for confining ultracold atoms in a trap by means of several techniques using various interactions (optical, magnetic, or electrostatic). This has renewed the interest in controlling Bose-Einstein condensates, few-body systems, or a single ion, trapped in or escaping from a time-dependent potential. The applications range from fundamental research to metrology and quantum information processing. Frequently, the manipulations involve externally controlled time-dependent Hamiltonians with both discrete and continuum levels. In some cases, the continuum is just a nuisance, leading to undesired atom loss, e.g., in the transport of trapped ions, or in trapped-ion atomic clocks. In other experiments the role of the continuum is essential in achieving, for example, outcoupling required in an atom laser with controlled atom flux [1,2], atomic pulses with a controlled velocity distribution [3], or constructing few-body number states [4–8]. A common feature of these techniques is the widespread use of adiabatic methods, where the potential is varied slowly in order to use the adiabatic phase, or to provide robust protocols, insensitive to systematic errors, that minimize the final excitation.

Similar considerations apply also to other fields, such as manipulation of electrons in semiconductor heterostructures, where the well depth or outcoupling control barriers are modified by potential gate voltages [9,10], or in harmonic generation, and internal atomic state preparation by intense laser pulses [11]. All this motivates the need to understand, and eventually control, "adiabaticity" when discrete levels are coupled to a continuum by the Hamiltonian time dependence. It is generally recognized that this is not a trivial task [12,13], since the textbook adiabaticity condition (AC), for a couple of discrete levels near an avoided crossing, is not directly applicable wherever a discrete level is coupled simultaneously to infinitely many δ-normalized continuum functions. Several authors have studied the bound-to-continuum adiabatic limit by analytical continuation, e.g., using Siegert states [14], Floquet resonances [11], and S-matrix poles [13].

The subject of this paper is somewhat narrower. We aim to study the adiabatic limit in the case where a discrete level approaches the continuum threshold, and then stops at some distance below it. Our model is an attractive δ-function potential, whose strength varies linearly with time. By employing the expansion in Sturmian eigenstates, we obtain an exact analytical solution, and use it to formulate the AC in terms of the level's final position and the speed at which it is moving. The condition, we argue, should provide guidance as to what can be expected in more complex systems and realistic potentials. The Sturmian technique has been developed in Refs. [15–18] for applications in the theory of atomic collisions. Similar approaches have been proven useful in the theory of Brownian motion [19], quantum measurements [20,21], and complex angular momentum analysis of integral [22,23] and differential [24,25] cross sections.

The rest of the paper is organized as follows. In Sec. II we estimate the loss of particles to the continuum by expanding the state of the system in the adiabatic basis. Section III describes our δ-function potential model. Section IV reviews its Sturmian eigenvalues and the associated analytical structure. In Sec. V we obtain the exact analytical solution for the wave function. In Sec. VI we formulate the appropriate adiabatic condition. In Sec. VII we use the Sturmian technique to analyze the AC for a zero range well confined in a box. Section VIII contains our conclusions.

II. ADIABATIC LIMIT FOR THE NONESCAPE PROBABILITY BY PERTURBATION THEORY

Consider a particle of mass μ in a one-dimensional potential well of a finite range. The potential changes with time in such a way that, when a particular bound state ϕ_0 attains certain energy, the evolution stops and we evaluate the probability for a particle to remain in the level, provided it was put there initially. Let the Hamiltonian (we use $\hbar = 1$ throughout this section)

$$H(t,v) = -\partial_x^2/2\mu + V(vt) \tag{1}$$

describe the evolution, whose speed is controlled by the parameter v and that starts at $t_i = 0$. For $v = 1$, at t_f it takes the chosen (ith) level to a desired depth within the modified well, $E_i(t_f) = E_i' < 0$. We wish to know the conditions for the particle, initially in the state i, to remain there at t_f. Assume, for simplicity, the well to be contained within a large box. Expanding the wave function in the discrete adiabatic basis,

$$H(t,v=1)\phi_n(t) = E_n(t)\phi_n(t), \tag{2}$$

we recover the standard adiabatic equations for the coefficients $a_m(t)$ which multiply $\phi_m(vt)\exp[-i\int_0^t E_m(vt')dt']$ [26],

$$\dot{a}_m(t/v) = -v\sum_{n\neq m}\frac{\langle\phi_m(t)|\dot{V}(t)|\phi_n(t)\rangle}{E_n(t)-E_m(t)} \times e^{-\frac{i}{v}\int_0^t[E_n(t')-E_m(t')]dt'}a_n(t/v). \quad (3)$$

These are to be solved with the initial condition (δ_{mi} is the Kronecker δ)

$$a_m(0) = \delta_{mi}. \quad (4)$$

In the near-adiabatic limit, $v\to 0$, replacing in the right-hand side (RHS) of Eq. (3) a_n with δ_{mi}, yields

$$a_{m\neq i}(t_f/v) = -\int_0^{t_f}\frac{\langle\phi_m(t')|\dot{V}(t')|\phi_i(t')\rangle}{E_i(t')-E_m(t')} \times e^{\frac{-i}{v}\int_0^{t'}[E_i(t'')-E_m(t'')]dt''}dt'. \quad (5)$$

Since the adiabatic levels cannot cross, the phase of the exponential in (5) does not have stationary points on the real axis, and as $v\to 0$, the leading contributions to the integral come from the end points, the times $t_i = 0$ and t_f, when the evolution is started and stopped. If the evolution is turned on gradually, or the initial well is so deep that the ith state is efficiently decoupled from the rest of the spectrum, the contribution from t_i can be neglected, and for the probability to leave the level by the time its energy is E_i' we have

$$\delta P_{\rm leave}(E_i',v) \equiv \sum_{m\neq i}|a_m(t_f/v)|^2 = v^2\sum_{m\neq i}\frac{|\langle\phi_m(t_f)|\dot{V}(t_f)|\phi_i(t_f)\rangle|^2}{|E_i(t_f)-E_m(t_f)|^4}+o(v^2). \quad (6)$$

Thus the adiabatic limit for the population of the ith level is reached provided

$$\delta P_{\rm leave}(E_i',v) \ll 1. \quad (7)$$

A simple example is given in Fig. 1, which shows the adiabatic spectrum of a potential $\Omega\delta(x)$ placed in a box with infinite walls at $x=\pm a$, as Ω increases from large negative to large positive values. A very deep δ well supports a bound state at $E_0\approx\Omega<0$, and divides the box $-a\leqslant x\leqslant a$ into two disjoint wells of a width a, each supporting the levels $E_m(\Omega=-\infty)=(m\pi/a)^2/2\mu>0$, $m=1,2,\ldots$. As Ω increases, E_0 moves upwards, and crosses the threshold $E=0$ for $\Omega=-1/a$. At the same time, symmetric positive energy states E_m also move upwards, while the antisymmetric states are unaffected. By the time $\Omega>0$ is so large that an impenetrable δ barrier divides the well, each positive-energy level will have moved one notch up, $E_m(\Omega=\infty)=[(m+1)\pi/a]^2/2\mu$, letting the former bound state of the δ-well occupy the symmetric ground state, $E_0(\Omega=\infty)=(\pi/a)^2/2\mu$.

As the box is made wider, $a\to\infty$, the positive energy levels become denser, and eventually form a continuum. In this case, the sums in Eqs. (3)–(6) must be replaced by integrals,

$$\delta P_{\rm leave}(E_i',v)\sim v^2\int_0^\infty\frac{|\langle\phi_k(t_f)|\dot{V}(t_f)|\phi_0(t_f)\rangle|^2}{|E_0(t_f)-k^2/2\mu|^4}dk, \quad (8)$$

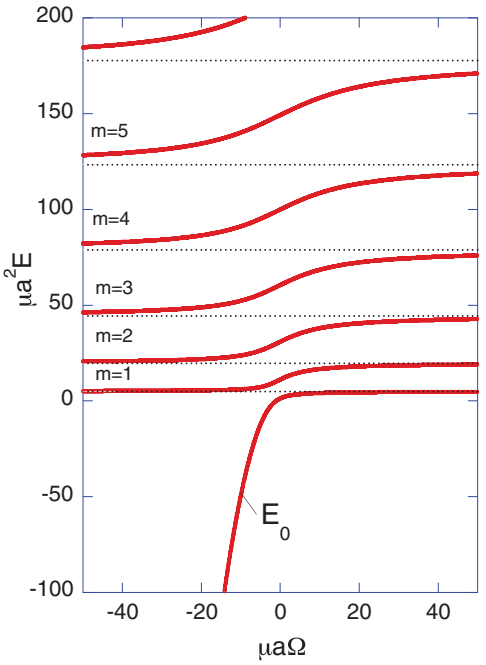

FIG. 1. (Color online) Spectrum of a potential $\Omega\delta(x)$ placed between infinite walls at $x=\pm a$ as a function of the potential strength Ω. The energies of symmetric states are shown by solid lines. The energies of antisymmetric states, unaffected by the δ potential, are indicated by dots.

where ϕ_k are the symmetric scattering states, $\phi_k(x)=\phi_k(-x)$, normalized by the condition $\langle\phi_k|\phi_{k'}\rangle=\delta(k-k')$.

Equations (6)–(8) have the advantage of giving a direct estimate of the loss of particles from a moving level, provided the loss is itself small. They contain, however, no information about the phase of the evolved state. Neither do they suggest a simple estimate for the degree of adiabaticity, based on the level's position and the speed at which the level is moving. We will look for such an estimate by considering an exactly solvable model.

III. LINEAR ZERO-RANGE MODEL

Consider, in one dimension, a particle of mass μ, trapped in a zero width well, $V(x)=W_0vt\delta(x)$, whose strength varies linearly with time. Scaling the variables, $x\to x/x_0$, $t\to t/t_0$, with $x_0=\hbar/\mu^{2/3}W_0^{1/3}$ and $t_0=\mu x_0^2\hbar$, we obtain the Schrödinger equation (SE)

$$i\partial_t\Psi(x,t) = -\partial_x^2\Psi/2 + vt\delta(x)\Psi, \quad (9)$$

in dimensionless variables x, t, and v. As the strength of the potential decreases, its single bound state at

$$E_0(t) = -v^2t^2/2 \equiv -\Omega^2(t)/2$$

moves ever closer to the continuum. At some t_f, $\Omega(t_f)=\Omega_f<0$ the evolution is halted, and we check on the state of the particle originally trapped in the bound state,

$$\phi_0(x,\Omega_f) = |\Omega_f|^{1/2}[\theta(x)\exp(-|\Omega_f|x) + \theta(-x)\exp(|\Omega_f|x)]. \quad (10)$$

[Here and below we use $\theta(x) = 1$ for $x > 0$, 0 for $x < 0$ and $\theta(0) = 1/2$.]

Thus we need to solve the SE (9) with the initial condition

$$\lim_{t\to-\infty}\Psi(x,t) \to \exp\left[-i\int_0^t E_0(t')dt'\right]\phi_0(x,\Omega). \quad (11)$$

Note that no generality has been lost by choosing the linear evolution, as long as one is interested in the level's population, and this level is close to the adiabatic regime. In this limit the RHS of Eq. (6) only depends on the time derivative of the potential at t_f, while the dynamical phases $\int_0^t [E_n(t') - E_m(t')]dt'$, which contain information about its previous history, cancel. To proceed with the solution of Eq. (9) we next define Sturmian eigenvalues and eigenfunctions.

IV. STURMIANS AND THEIR ANALYTIC STRUCTURE

To define the Sturmian basis required in what follows, we first take the Fourier transform of Eq. (9) with respect to time. We then fix the energy ω and look for a (possibly complex-valued) potential strength $\rho(\omega)$, such that the Schrödinger equation (SE),

$$\omega S(x,\omega) = -\partial_x^2 S/2 + \rho(\omega)\delta(x)S, \quad (12)$$

has a solution, which for $\omega > 0$ contains only outgoing waves emitted from the origin,

$$S(x,\omega) = [\theta(x)\exp(i\sqrt{2\omega}x) + \theta(-x)\exp(-i\sqrt{2\omega}x)]. \quad (13)$$

We choose to normalize the solution by the condition $S(0,\omega) = 1$. Equations (12) and (13) define a Sturm-Liouville problem, with a Sturmian eigenvalue $\rho(\omega)$ and the corresponding Sturmian eigenfunction $S(x,\omega)$, which, following Refs. [15], we will call simply Sturmian. Typically, the boundary conditions allow for only discrete values of ρ.

Our case is particularly simple: there is only one Sturmian per zero-range potential (see, for example [18]). Indeed, the presence of the Dirac δ in Eq. (12) requires that the log derivative of $S(x,\omega)$ jump at $x = 0$ by 2ρ. Thus we have

$$\rho(\omega) = i\sqrt{2\omega}. \quad (14)$$

For an energy ω, real or complex valued, Eqs. (13) and (14) define $\rho(\omega)$ and $S(x,\omega)$, both single valued on the two-sheet Riemann surface $\mathcal{R}$ cut along the real ω axis (see Fig. 2). On the first sheet of $\mathcal{R}$, with negative energy, $\omega < 0$, the Sturmian coincides (up to a normalization) with the adiabatic bound state [cf. Eq. (10)],

$$\phi_0(x,\Omega(t)) = |\Omega|^{1/2}S(x, -\Omega^2/2). \quad (15)$$

For $\omega > 0$, just above the cut, we have $i\sqrt{2\omega} = i|\sqrt{2\omega}|$, and $S(x,\omega)$ contains only the waves propagating away from the origin. This requires an emitting potential at $x = 0$, which is the case since $\rho(\omega) = i|\sqrt{2\omega}|$. Just below the cut we have only incoming waves converging on the origin, $i\sqrt{2\omega} = -i|\sqrt{2\omega}|$, and an absorbing potential $-i|\sqrt{2\omega}|\delta(x)$.

Also present in Fig. 2 are the Siegert states [14], defined as the solutions of the SE (12) satisfying, for a real potential strength ρ, the "outgoing boundary condition" with a complex wave number $k(\rho) = -i\rho$,

$$s(x,\rho) = \{\theta(x)\exp[ik(\rho)x] + \theta(-x)\exp[-ik(\rho)x]\}. \quad (16)$$

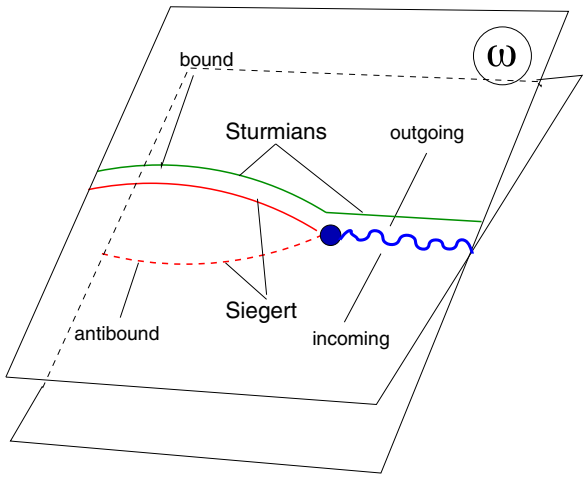

FIG. 2. (Color online) Two-sheet Sturmian Riemann surface of $\rho(\omega)$ cut along the positive real axis. The Sturmians used in Eq. (24) lie on the contour following the real axis above the cut on the first sheet. The states above and below the cut contain only outgoing and incoming waves, respectively. The Siegert states lie on the negative semiaxis of the first and the second sheet, where they correspond to the bound and antibound states of the δ well, respectively.

These can be found by following on $\mathcal{R}$ the path $\mathrm{Im}\rho(\omega) = 0$, which runs up the negative semiaxis on the first sheet to the branching point, and then continues down the negative semiaxis on the second sheet (see Fig. 2). There is only one Siegert state for each potential strength. On the first sheet such a state coincides (up to a normalization) with the adiabatic bound state (10), while on the second sheet it becomes an antibound state which grows exponentially as $|x| \to \infty$.

Alternatively, one can use the potential strength ρ as the independent variable, thus defining for each ρ the energy $\omega(\rho)$

$$\omega(\rho) = -\rho^2/2 \quad (17)$$

and the Sturmian $S(x,\omega(\rho))$, both single valued in the complex ρ plane. In this plane the real-energy Sturmians (13) lie along the contour consisting of positive real and positive imaginary semiaxis, while the Siegert states inhabit all of the real ρ axis.

We note that in this case the use of the Siegert states, e.g., by the method developed in [14], is problematic, since the width of the inner region of the well, where the Siegert expansion is performed, is zero. The use of the real energy Sturmians allows us, however, to obtain a simple analytic solution.

V. SOLUTION

Following [15] to solve the SE (9), we change to the energy representation

$$\omega\Psi(x,\omega) = -\partial_x^2\Psi/2 - iv\delta(x)\partial_\omega\Psi, \quad (18)$$

where

$$\Psi(x,t) = \int d\omega\, \exp(-i\omega t)\Psi(x,\omega), \quad (19)$$

and make the *ansatz*

$$\Psi(x,\omega) = B(\omega)S(x,\omega), \quad (20)$$

where the coefficients $B(\omega)$ are to be determined. There is a physical reason for choosing the set of all $S(x,\omega)$ with outgoing boundary conditions. At any time there may only be particles emitted from the rising bound state, and the Sturmians cover all such possibilities. Inserting (20) into (18) and then adding and subtracting $\rho(\omega)\delta(x)B(\omega)S(x,\omega)$ in its RHS yields

$$[iv\delta(x)\partial_\omega + \rho(\omega)\delta(x)]B(\omega)S(x,\omega) = 0, \tag{21}$$

so that after integrating over x we have

$$iv\partial_\omega B + \rho B(\omega) = 0, \tag{22}$$

and, explicitly,

$$B(\omega) = C\,\exp\left[\frac{i}{v}\int_0^\omega \rho(\omega')d\omega'\right] = C\,\exp\left(-\frac{2^{3/2}\omega^{3/2}}{3v}\right), \tag{23}$$

where C is a yet unknown constant. We then have

$$\Psi(x,t) = C\int d\omega\,\exp\left(-i\omega t - \frac{2^{3/2}\omega^{3/2}}{3v}\right)S(x,\omega), \tag{24}$$

where the integration contour runs above the cut on the first sheet of the Riemann surface $\mathcal{R}$ shown in Fig. 1. The value of C,

$$C = (2\pi i v)^{-1/2}, \tag{25}$$

is determined by sending $t \to -\infty$, evaluating the integral in (24) by the stationary phase (SP) method, and comparing the result with the initial condition (11) (for details, see the Appendix).

Note that we have avoided solving the coupled equations (3), and obtained the exact solution of Eq. (9) in a form of single quadrature (24). We will further comment on this advantage of the Sturmian representation (20) in Sec. VII. Next we use Eq. (24) in order to evaluate the adiabatic condition.

VI. ADIABATIC LIMIT FOR THE NONESCAPE AMPLITUDE BY A STURMIAN EXPANSION

The amplitude to remain in the bound state whose energy is $E_f = -\Omega_f^2/2 < 0$ at a time t_f,

$$A_{\rm stay}(E_f,v) \equiv \langle\phi_o|\Psi(t)\rangle, \tag{26}$$

can now be written as an integral

$$A_{\rm stay}(E_f,v) = (2\pi i v)^{-1/2}\int_{-\infty}^{\infty} d\omega\,\exp\left[\frac{i}{v}\left(\omega\sqrt{2|E_f|} - \frac{2^{3/2}\omega^{3/2}}{3i}\right)\right]g(\omega,E_f), \tag{27}$$

where the overlap between the bound state and a Sturmian, $g(\omega,E_f) \equiv \langle\phi_o|S(\omega)\rangle$ is given by

$$g(\omega,E_f) = \frac{2|2E_f|^{1/4}}{|2E_f|^{1/2} - i(2\omega)^{1/2}}. \tag{28}$$

The probabilities to stay in the bound state are shown in Fig. 3 for various values of v. The integral has a SP point at $\omega_s = E_f$,

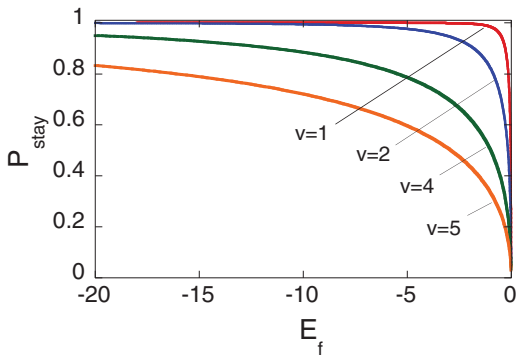

FIG. 3. (Color online) Probability to remain in the bound state of the δ well as a function of the final dimensionless energy $E_f = -vt_f^2/2t_0^2$ for various values of v. The amplitude $A_{\rm stay}(E_f,v)$ is obtained by evaluating the integral (27) along a suitable contour in the complex ω plane.

and the stationary phase result corresponds to the adiabatic limit,

$$A_{\rm stay}^{\rm adiab}(E_f,v) \sim \exp\left[-i\int_0^{t_f} E_0(t')dt'\right], \quad v \to 0, \quad \forall E_f < 0. \tag{29}$$

Thus, no matter how close the level approaches the threshold $E = 0$, it is possible to find an evolution slow enough for the wave function to follow it adiabatically. This is the *adiabatic theorem*.

One may ask a different question: given the values of v and E_f, will the adiabatic result (29) hold? For the primitive SP approximation (29) to be accurate, the stationary phase point should be well isolated from all singularities of the integrand of (28). That is, the width of the stationary region, $\Delta\omega_s$, should be much smaller than the distance from $\omega_s = E_f$ to the branching point at $\omega = 0$. From Eq. (A1), $\Delta\omega_s$ is just the square root of the level's velocity at $t = t_f$,

$$\Delta\omega_s \sim \left[v/\frac{d\rho(\omega_s)}{d\omega}\right]^{1/2} = \sqrt{\dot{E}_0(t_f)}. \tag{30}$$

Squaring the ratio $\Delta\omega_s/\omega_s$ we may say that the adiabatic approximation for $A_{\rm stay}$ is unlikely to be accurate unless the speed, with which the level moves just before it stops, is much smaller than the square of its final energy, i.e., unless [27]

$$\gamma \equiv \dot{E}_f/E_f^2\big|_{t=t_f} = 4v/\Omega_f^3 \ll 1. \tag{31}$$

The validity of Eq. (29) is illustrated in Fig. 4(a) showing the relative errors of the adiabatic approximation (29) as the function of the parameter γ for $v = 1$.

However, Fig. 4(a) also shows that the condition (31), which ensures adiabaticity for both the phase and the modulus of $A_{\rm stay}$, may be too strict for someone interested only in the probability to remain in the bound state, $P_{\rm stay} = |A_{\rm stay}|^2$. This is because the phase of $A_{\rm stay}$ becomes affected by the evolution earlier than its modulus $|A_{\rm stay}|$, which can remain close to unity for longer. Obtaining corrections to $|A_{\rm stay}|$ from the oscillating integral (27) is cumbersome [28], and to estimate $P_{\rm stay}$ we return to Eq. (8). The results are shown in Fig. 4(b). For our

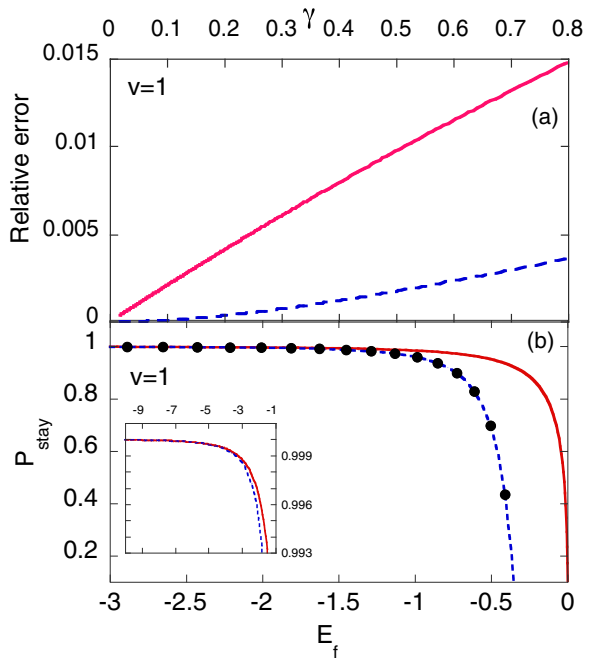

FIG. 4. (Color online) (a) Relative errors of the adiabatic approximation (29) vs γ in Eq. (31) for a δ potential in free space: $|A_{\rm stay} - A_{\rm stay}^{\rm adiab}|/|A_{\rm stay}|$ (solid) and $(|A_{\rm stay}^{\rm adiab}| - |A_{\rm stay}|)/|A_{\rm stay}|$; (b) same as Fig. 3 for $v = 1$. Shown are the exact probability in Eq. (27) (solid), its quadratic approximation (6) (dashed), and the curve $0.0195 \times (\dot{E}_0/E_0^2)^2|_{t=t_f}$ (filled dots). In the inset the region of validity of the quadratic approximation (6) is magnified for better viewing.

simple model we find ($v = 1$)

$$P_{\rm stay}(E_f, v) \approx 1 - C\gamma^2, \tag{32}$$

where $C \approx 0.0195$. Equation (32) correctly describes the loss of particles to the continuum to within 0.1%–0.2%, and after that it overestimates the probability of nonadiabatic transitions. Where Eq. (32) fails, the correct loss of particles to the continuum can be evaluated by constructing a uniform asymptotic approximation for the integral (32), allowing for coalescence of ω_s and the branching point at $\omega = 0$. We will not pursue this task further, and continue with another example, providing an additional insight into the benefits of the method.

VII. ZERO-RANGE WELL IN A BOX

Next we put a δ well at $x = 0$ inside a potential box with infinite walls at $x = \pm a$

$$V(x) = v t\delta(x) + W\theta(x - a) + W\theta(x + a), \quad W \to \infty. \tag{33}$$

The setup can be seen as a crude model of a narrow potential well inside an anharmonic trap, which can be constructed for cold atoms [2]. Rescaling the variables ($\hbar = 1$, $\mu = 1$),

$$x \to x/a, \quad t \to t/2a^2, \quad v \to 4a^3 v, \quad a \to 1, \tag{34}$$

allows us to consider the box of width equal to 2 for various values of the speed v. As before, we will assume that the evolution stops at some $E_f < 0$ ($\Omega_f < -1/a$), and evaluate the probability to remain in the negative energy bound state, $[\phi_0(x, E_f) = \phi_0(-x, E_f)]$,

$$\phi_0(x \geqslant 0, E_f) = N^{-1/2}(E_f)\left\{\exp\left[-\sqrt{2|E_f|}(x - a)\right] - \exp\left[\sqrt{2|E_f|}(x - a)\right]\right\}, \tag{35}$$

where $N(E_f) \equiv \langle\phi_0(E_f)|\phi_0(E_f)\rangle$ is the normalization constant.

Now a Sturmian eigenstate [we need to consider only those symmetric about the origin, $S(x) = S(-x)$] must vanish at $x = \pm a$, and at $x = 0$ its logarithmic derivative should jump by $\rho(\omega)$. We, therefore, have

$$\rho(\omega) = -k\,\cot(ka), \quad k \equiv \sqrt{2\omega}, \tag{36}$$

and

$$S(x \geqslant 0, \omega) = (e^{-ika} - e^{ika})^{-1} \times \{e^{ik(x-a)} - e^{-ik(x-a)}\}. \tag{37}$$

Expanding the wave function in $S(x,\omega)$ as in Eq. (20), and repeating the steps of Sec. V, for the amplitude to stay in $\phi_0(x, E_f)$ we obtain

$$A_{\rm stay}(E_f, v) = (2\pi i v)^{-1/2} \int_\Gamma d\omega \langle\phi_0(E_f)|S(\omega)\rangle \times \exp\left\{-\frac{i}{v}\left[\omega\Omega' - \int_0^\omega \rho(\omega')d\omega'\right]\right\}, \tag{38}$$

where $\langle\phi_0(E_f)|S(\omega)\rangle \equiv \int_{-a}^{a} \phi_0(x, \Omega')S(x,\omega)dx$.

The choice of the contour Γ, which must run above the positive real axis, may require an explanation. Both $\rho(\omega)$ and $S(x,\omega)$ are single valued in the complex ω plane, and have poles on the real ω axis at the energies corresponding to the box divided in two by an infinite δ well or barrier, $\omega_m = (m\pi/a)^2/2$, $m = 1, 2, \ldots$. (There Sturmians vanish at $x = 0$, and an infinite ρ is required to ensure the correct discontinuity in their log derivatives.) In the limit of the broad box, $a \to \infty$, the poles merge into a cut shown in Fig. 2. Above the cut we have $k(\omega + i\epsilon) \sim \sqrt{2\omega} + i\epsilon'$, and recover Eqs. (12) and (13) obtained in the continuum case,

$$\rho(\omega + i\epsilon) \sim i\sqrt{2\omega}, \quad S(x \geqslant 0, \omega + i\epsilon) \sim \exp(i\sqrt{2\omega}x), \quad \text{as} \quad a \to \infty, \quad \epsilon \to +0, \tag{39}$$

provided Γ runs along the negative and above the positive ω axis.

Equation (36) provides some insight into the advantage offered by the Sturmian representation (20). There is only one (real) value of the potential strength ρ for a given real energy ω (cf. Fig. 1). Conversely, for each value of ρ there are infinitely many values of ω, corresponding to different branches of the inverse cotangent. These are seen as different energy levels in Fig. 1, and give rise to an infinite number of coupled equations in Eq. (3) if we choose to expand the wave function in the adiabatic basis (2) defined for each potential strength. If, on the other hand, we choose energy as the independent variable, there is only one state $S(\omega)$ in which to expand, and a single equation (22), which later yields the analytical expressions (27) and (38).

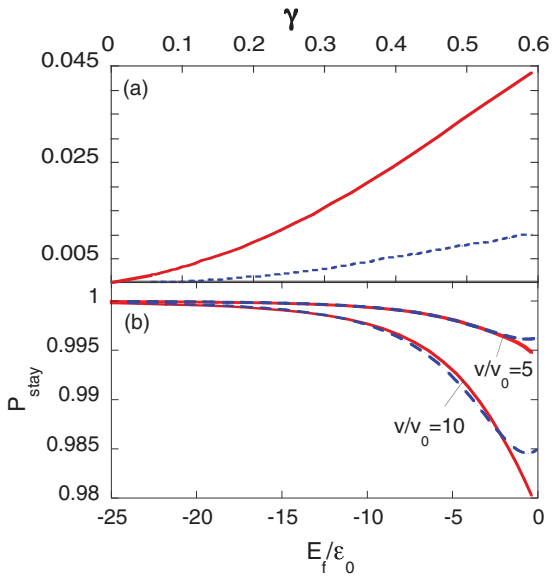

FIG. 5. (Color online) (a) Relative errors of the adiabatic approximation (29) as a function of the parameter γ in Eq. (31) for a δ potential in a box of unit half-width: $|A_{\rm stay} - A^{\rm adiab}_{\rm stay}|/|A_{\rm stay}|$ (solid) and $(|A^{\rm adiab}_{\rm stay}| - |A_{\rm stay}|)/|A_{\rm stay}|$; (b) the probability to stay in the bound state of a δ well approaching the threshold $E = 0$ for $v/v_0 = 5$ and 10, vs E_f/ϵ_0, where $v_0 \equiv 1/4a^3$ and $\epsilon_0 \equiv 1/2a^2$. Shown are the exact probability in Eq. (27) (solid), and its quadratic approximation (6) (dashed). The amplitude $A_{\rm stay}(E_f, v)$ is obtained by evaluating the integral (38) along a suitable contour in the complex ω plane.

As in Sec. VI, the adiabatic limit for the amplitude $A_{\rm stay}(E_f, v)$ is achieved provided the integral (38) is correctly evaluated by the primitive SP approximation described in the Appendix. This requires a sufficient separation between the stationary phase region and the nearest singularity, the pole at $\omega_1 = \pi^2/2a^2$, i.e., provided

$$\gamma \equiv \dot{E}_f/(\omega_1 - E_f)^2 \ll 1. \tag{40}$$

Relative errors of the adiabatic approximation for different values of γ are shown in Fig. 5(a).

As in Sec. VI the condition (40) does not, alone, provide an estimate for $P_{\rm stay}$. This probability can be evaluated by noting that for the parameters used in Fig. 5, the nonadiabatic transitions occur only between the two lowest states in the spectrum shown in Fig. 1. Restricting the summation in Eq. (6) to the first ($m = 1$) term only, we have

$$P_{\rm stay} \approx 1 - \gamma^2 \left(\frac{\omega_1 - E_f}{E_1(t_f) - E_f} \right)^4 \left| \frac{\phi_1(x = 0, t_f)}{\phi_0(x = 0, t_f)} \right|^2. \tag{41}$$

The probability to leave the level vanishes, as it should as $\gamma \to 0$. In addition, it is reduced by the fourth power of the ratio $(\omega_1 - E_f)/[E_1(t_f) - E_f]$, which is always less than unity, since $E_1(t_f) > \omega_1$ (cf. Fig. 1). The values of $P_{\rm stay}$ and its two-level approximation (41) are shown in Fig. 5(b).

VIII. CONCLUSIONS AND DISCUSSION

In summary, the Sturmian representation allows one to express the amplitude to remain in the initial bound state of a time-dependent well, $A_{\rm stay}$, in the form of an oscillating integral over the energy domain. The integrand has a stationary region whose center coincides with the energy E_0 of the adiabatic state. The width of the region is determined by the speed $\dot{E}_0$, with which the level moves as the potential changes. The adiabatic limit is reached provided the integral can be accurately evaluated by the primitive stationary phase approximation. This happens when the stationary region is well separated from the nearest singularity of the integrand at some $E_{\rm sing}$, i.e., provided

$$\gamma = \hbar \dot{E}_0/|E_0 - E_{\rm sing}|^2 \ll 1. \tag{42}$$

In the case of a continuum, the relevant singularity is the branching point at the origin, $E_{\rm sing} = 0$. The condition $\gamma \ll 1$ is, therefore, necessary for both the phase and the modulus of $A_{\rm stay}$ to reach the adiabatic limit.

There are, however, at least two reasons why the condition (42) may prove to be too strict. First, it does not specify how quickly the error will grow, as γ increases. This depends on the type of the singularity, and must be determined by evaluating the uniform asymptote of the corresponding oscillatory integral, allowing the singularity to coalesce with the stationary point. Figure 3(a) shows that this growth is slow when the singularity is of the weak branching type. The growth is faster for a stronger pole singularity, as is shown in Fig. 5(a).

Secondly, Eq. (42) may be too strict for someone interested, for example, only in the probability to remain in the adiabatic state, $P_{\rm stay} = |A_{\rm stay}|^2$. Figures 3(a) and 4(a) show that the phase of $A_{\rm stay}$ is more sensitive to the motion of the level than its modulus, and $P_{\rm stay}$ may remain close to unity even after the adiabatic approximation for the phase has failed. Again, obtaining the exact adiabatic condition for $P_{\rm stay}$ requires an analysis of the integral for $A_{\rm stay}$ beyond the primitive SP approximation.

Although in this paper we analyzed the exactly solvable model, where only one Sturmian is required for expanding the wave function $|\Psi(t)\rangle$, one may expect the above conclusions to apply also to more realistic potentials. For example, in the case of a well of a finite width, there are infinitely many Sturmians in the expansion of $|\Psi(t)\rangle$. However, in the near-adiabatic limit, only one Sturmian state remains populated, giving rise to integrals similar to (27) and (38). A detailed analysis will be given in our future work.

Finally, we note that if the potential's evolution is not linear in time, but sufficiently slow for Eq. (6) to hold, the condition $\gamma \ll 1$ would guarantee that $P_{\rm stay} \approx 1$, although it would almost certainly be too strict in the sense explained above.

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APPENDIX: DERIVATION OF EQ. (25)

In the energy variable ω the Taylor expansion for the phase $\Phi(\omega)$ of the exponential in the integral (24) around its

stationary point ω_s, defined by $\rho(\omega_s) = vt$, takes the form

$$\Phi(\omega) = -\omega_s t + v^{-1}\int_0^{\omega_s} \rho(\omega')d\omega' + v^{-1}\sum_{n=2}^{\infty} \frac{\rho^{(n-1)}(\omega_s)}{n!}(\rho-\rho_s)^n. \quad \text{(A1)}$$

Changing to the ρ variable as discussed in Sec. IV we obtain an equivalent form of Eq. (24),

$$\Psi(x,t) = C\left\{\int_{-\infty}^{0} + \int_0^{i\infty}\right\}d\rho \times \frac{d\omega}{d\rho}\exp\left[i(\rho/v - t)\omega - \frac{i}{v}\int_0^{\rho}\omega(\rho')d\rho'\right] S(x,\omega). \quad \text{(A2)}$$

For a large negative t, the phase of the exponential in the first integral, $\Phi(\rho)$, has a stationary phase point $\rho_s = vt$, In its vicinity we have

$$\Phi(\rho) = -\int_0^t E_0(t')dt' + v^{-1}\sum_{n=2}^{\infty}\frac{(n-1)}{n!}\frac{d^{n-1}\omega(\rho_s)}{d\rho^{n-1}}(\rho-\rho_s)^n, \quad \text{(A3)}$$

where the first term coincides with the adiabatic phase in Eq. (11). Evaluating the stationary phase result,

$$\Psi(x,t) \sim \exp\left[-i\int_0^t E_0(t')dt'\right] \times\sqrt{\frac{2\pi}{-i\,\Phi''(\rho_s)}}\frac{d\omega(\rho_s)}{d\rho}S(x,\rho_s) \quad \text{(A4)}$$

for $t \to -\infty$, and recalling from Eqs. (10), (13), and (17) that $\phi_0(x,t) = \sqrt{d\omega(\rho_s)/d\rho}\; S(x,\omega(\rho_s))$, we obtain Eq. (25).

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[26] Note that there is no phase term $\langle\phi_m|\dot{\phi}_m\rangle$ (i.e., we use "parallel transport") as the bound states in a one-dimensional box can alway be chosen real.

[27] The importance of the ratio $\dot{E}_f/E_f^2$ could have been guessed, since it is the only dimensionless parameter involving both the velocity and the position of the moving level. We did, however, clarify the origin of the estimate (31).

[28] One may proceed by expanding the integral (27) in an asymptotic series in powers v. A more detailed analysis shows that the leading corrections come from the vicinity of the branching point $\omega = 0$. There the integral (27) expands in powers of $v^{1/6}$, and collecting all terms, many of which cancel, to the order of v^2 is indeed cumbersome.