

Escape behavior of a quantum particle in a loop coupled to a lead

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(Received 14 October 2011; published 29 December 2011)

We consider a one-dimensional loop of circumference L crossed by a constant magnetic flux Φ and connected to an infinite lead with coupling parameter ε . Assuming that the initial state ψ_0 of the particle is confined inside the loop and evolves freely, we analyze the time evolution of the nonescape probability $P(\psi_0, L, \Phi, \varepsilon, t)$, which is the probability that the particle will still be inside the loop at some later time t . In appropriate units, we found that $P(\psi_0, L, \Phi, \varepsilon, t) = P_\infty(\psi_0, \Phi) + \sum_{k=1}^{\infty} C_k(\psi_0, L, \Phi, \varepsilon)/t^k$. The constant $P_\infty(\psi_0, \Phi)$ is independent of L and ε , and vanishes if ψ_0 has no bound state components or if $|\cos(\Phi)| \neq 1$. The coefficients $C_1(\psi_0, L, \Phi, \varepsilon)$ and $C_3(\psi_0, L, \Phi, \varepsilon)$ depend on the initial state ψ_0 of the particle, but only the momentum $k = \Phi/L$ is involved. There are initial states ψ_0 for which $P(\psi_0, L, \Phi, \varepsilon, t) \sim C_\delta(\psi_0, L, \Phi, \varepsilon)/t^\delta$, as $t \rightarrow \infty$, where $\delta = 1$ if $\cos(\Phi) = 1$ and $\delta = 3$ if $\cos(\Phi) \neq 1$. Thus, by submitting the loop to an external magnetic flux, one may induce a radical change in the asymptotic decay rate of $P(\psi_0, L, \Phi, \varepsilon, t)$. Interestingly, if $\cos(\Phi) = 1$, then $C_1(\psi_0, L, \Phi, \varepsilon)$ decreases with ε (i.e., the particle escapes faster in the long run) while in the case $\cos(\Phi) \neq 1$, the coefficient $C_3(\psi_0, L, \Phi, \varepsilon)$ increases with ε (i.e., the particle escapes slower in the long run). Assuming the particle to be initially in a bound state of the loop with $\Phi = 0$, we compute explicit relations and present some numerical results showing a global picture in time of $P(\psi_0, L, \Phi, \varepsilon, t)$. Finally, by using the pseudospectral method, we consider the interacting case with soft-core Coulomb potentials.

DOI: [10.1103/PhysRevA.84.062126](https://doi.org/10.1103/PhysRevA.84.062126)

PACS number(s): 03.65.Db, 03.65.Nk

I. INTRODUCTION

The study of open quantum systems has attracted many researchers in theoretical physics during the last decades and is still under intense investigation. One of the most basic problems in this field is to understand how a quantum particle initially confined inside an open cavity will escape (see, e.g., [1] for a general discussion). In the literature, such systems are commonly described in terms of the following quantities: the *nonescape probability* $P(t)$, which is the probability that the particle will still be inside the cavity at some later time t , and the *survival probability* $S(t)$, which is the probability of finding the particle in the initial state at time t [2]. Let us suppose that the configuration space is the one-dimensional (1D) half-line $[0, \infty)$ and that the cavity is the interval $[0, L]$. Then, at time $t = 0$, the particle is supposed to be in a normalized state ψ_0 satisfying $\psi_0(x) = 0$ for all $x \notin [0, L]$. If H denotes the Hamiltonian of the particle and $\psi(x, t) = (e^{-iHt/\hbar}\psi_0)(x)$ its state at time $t > 0$, where \hbar is the reduced Planck constant, then the nonescape and survival probabilities are given by

$$P(t) = \int_0^L \overline{\psi(x, t)} \psi(x, t) dx, \quad (1)$$

$$S(t) = \left| \int_0^L \overline{\psi_0(x)} \psi(x, t) dx \right|^2, \quad (2)$$

where the overbar denotes complex conjugation. It is easy to check that these quantities satisfy $S(0) = P(0) = 1$ and $0 \leq S(t) \leq P(t) \leq 1$ for all times $t > 0$. Although both quantities are interesting, we shall discuss only $P(t)$ in this paper. Note, however, that by analyzing the time decay of $P(t)$ one automatically gets an upper bound for $S(t)$.

The nonescape probability $P(t)$ has been discussed in free 1D quantum systems [3], in free two-dimensional (2D) quantum billiard systems [4,5], and also in three-dimensional (3D) quantum systems with finite range potentials [6]. Interestingly, if the initial state ψ_0 has no bound state components, then it is always found that the long-time behavior of $P(t)$ is a power law: $P(t) = C/t^\delta + O(1/t^{\delta+1})$ as $t \rightarrow \infty$, where the constant C and the exponent δ depend on the geometry of the system and on the initial state ψ_0 of the particle. Some readers may be surprised since it is well known that various spontaneous decays have been observed to follow an exponential law. This apparent discrepancy may actually be only a time-scale problem. Indeed, although quantum mechanics clearly predicts in general some deviation from exponential decay, the following phases may well occur [7–9]: for a short time the decay is parabolic $P(t) = 1 - ct^2$, then it is approximately exponential and finally becomes a power-law at very large times.

In the present paper, we consider the model introduced in [10] in which the cavity is a one-dimensional loop $[0, L]$ crossed by a constant magnetic flux Φ and connected, with coupling parameter ε , to an infinite one-dimensional lead $[L, \infty)$ (the points $x = 0$ and $x = L$ are identified), so that the particle may escape freely from the loop; see Fig. 1. This model contains rich physics and is simple enough to be amenable by analytical means or numerical simulations, and thus has been the subject of several works [10–18]. Nevertheless, the nonescape probability $P(\psi_0, L, \Phi, \varepsilon, t)$ has never been discussed in this model and it is interesting to know precisely how it depends on the initial state ψ_0 of the particle and on the three physical parameters: the loop's length L , the external magnetic flux Φ , and the coupling ε .

In appropriate units, here is a summary of our main results.

(1) Let $\lambda > 0$, then one has the following scaling law:

$$P(\psi_0, \lambda L, \Phi, \varepsilon, t) = P\left(\psi_0, L, \Phi, \varepsilon, \frac{t}{\lambda^2}\right). \quad (3)$$

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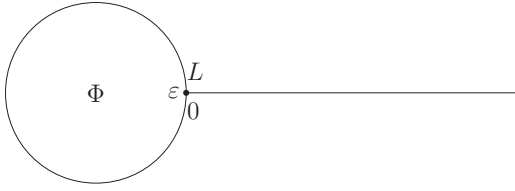


FIG. 1. A loop connected to a lead.

Thus, increasing, for example, the length of the loop by a factor $\lambda = 2$ leads to a nonescape probability evolving $\lambda^2 = 4$ times slower.

(2) The nonescape probability may be written as

$$P(\psi_0, L, \Phi, \varepsilon, t) = P_\infty(\psi_0, \Phi) + \sum_{k=1}^{\infty} \frac{C_k(\psi_0, L, \Phi, \varepsilon)}{t^k}. \quad (4)$$

The constant $P_\infty(\psi_0, \Phi)$ is given in (58): It is independent of L and ε , and vanishes if ψ_0 has no bound state components or if $|\cos(\Phi)| \neq 1$. In the infinite series, the leading term always has an odd power. The coefficients $C_1(\psi_0, L, \Phi, \varepsilon)$ and $C_3(\psi_0, L, \Phi, \varepsilon)$ are given in (66)–(68): They depend on the initial state ψ_0 of the particle, but only the momentum $k = \Phi/L$ is involved. When $\Phi = 0$, this coincides with the well-known fact that only the zero momentum of ψ_0 plays a role in the long-time behavior of the nonescape probability [3]. If $\cos(\Phi) = 1$, then there are initial states ψ_0 with no bound state components [e.g., (85)] for which $C_1(\psi_0, L, \Phi, \varepsilon) \neq 0$, while the coefficients $C_1(\psi_0, L, \Phi, \varepsilon)$ and $C_2(\psi_0, L, \Phi, \varepsilon)$ always vanish if $\cos(\Phi) \neq 1$. The important consequence is that there are initial states ψ_0 giving a power law decay:

$$P(\psi_0, L, \Phi, \varepsilon, t) = \frac{C_\delta(\psi_0, L, \Phi, \varepsilon)}{t^\delta} + O\left(\frac{1}{t^{\delta+1}}\right), \quad (5)$$

where $\delta = 1$ if $\cos(\Phi) = 1$ and $\delta = 3$ if $\cos(\Phi) \neq 1$. In particular, we see that by submitting the loop to an external magnetic flux (thus going from $\Phi = 0$ to $\Phi \neq 0$), one may induce a radical change in the decay rate of $P(\psi_0, L, \Phi, \varepsilon, t)$. If $\cos(\Phi) = 1$, then $C_1(\psi_0, L, \Phi, \varepsilon)$ decreases with ε (i.e., the particle escapes faster in the long run) and if $\cos(\Phi) \neq 1$, then $C_3(\psi_0, L, \Phi, \varepsilon)$ increases with ε (i.e., the particle escapes slower in the long run). Interestingly, similar features were obtained in a circular dielectric cavity containing classical waves [19], the nature of the waves (TM or TE) and the refractive index of the cavity playing a similar role to Φ and ε .

(3) Assuming the particle to be initially in a bound state of the loop with $\Phi = 0$ [see (72)], we computed explicitly $P_\infty(\psi_0, \Phi)$, $C_1(\psi_0, L, \Phi, \varepsilon)$, and $C_3(\psi_0, L, \Phi, \varepsilon)$ [see (73)–(76)]. As one may expect, we found that higher energetic bound states decay faster. Interestingly, we observed that the coefficient $C_3(\psi_0, L, \Phi, \varepsilon)$ oscillates, nonperiodically, with Φ ; see Fig. 5. We also present some numerical results showing a global picture in time of $P(\psi_0, L, \Phi, \varepsilon, t)$; see Figs. 6–10. They reveal in particular that if $\cos(\Phi) \neq 1$, then by increasing the value of ε , the particle escapes faster in the beginning but slower in the long run as stated previously.

This paper is organized as follows. In Sec. II, we model the situation depicted in Fig. 1 in the framework of standard quantum mechanics. In the paper [10], the scattering processes

occurring at the connecting point (between the loop and the lead) are described in terms of an energy-independent scattering matrix S . We shall show that this scattering matrix may be used to prescribe boundary conditions at the connecting point for which the Hamiltonian of the particle is self-adjoint. In Sec. III, we solve the time-dependent Schrödinger equation and derive its associated propagator. We then analyze the long-time behavior of the propagator and consequently that of the nonescape probability. We discuss our general results in Sec. IV and consider some particular initial states in Sec. V. In Sec. VI, we present an interesting and highly nontrivial application of the pseudospectral method by considering the interacting case with soft-core Coulomb potentials. Finally, in Sec. VII we make some concluding remarks.

II. THE HAMILTONIAN

In standard quantum mechanics, the situation depicted in Fig. 1 is modeled as follows: The physical states of the particle belong to the Hilbert space $\mathcal{H} = L^2([0, L]) \oplus L^2([L, \infty))$ and the Hamiltonian of the particle reads [10]

$$H = \left[-i \frac{d}{dx} - \frac{\Phi}{L} \chi_{[0, L]}(Q) \right]^2, \quad (6)$$

where $\chi_{[0, L]}(Q)$ is the operator of multiplication by $\chi_{[0, L]}(x)$, where $\chi_{[0, L]}(x) = 1$ if $x \in [0, L]$ and $\chi_{[0, L]}(x) = 0$ otherwise. Here we have set $\hbar = 1$ for the reduced Planck constant, $e = 1$ for the electric charge, $c = 1$ for the speed of light, and $m = 1/2$ for the mass of the particle.

Let ψ be a state in \mathcal{H} , then it can be uniquely written as $\psi = \psi_{\text{LOOP}} + \psi_{\text{LEAD}}$, with $\psi_{\text{LOOP}} \in L^2([0, L])$ and $\psi_{\text{LEAD}} \in L^2([L, \infty))$. To simplify the notations, we shall use the following convention: $\psi(x) = \psi_{\text{LOOP}}(x)$ if $x \in (0, L)$, $\psi(x) = \psi_{\text{LEAD}}(x)$ if $x \in (L, \infty)$ and $\psi(0_+) = \psi_{\text{LOOP}}(0)$, $\psi(L_-) = \psi_{\text{LOOP}}(L)$, $\psi(L_+) = \psi_{\text{LEAD}}(L)$.

The Hamiltonian H is an unbounded operator and thus cannot be defined on the entire Hilbert space \mathcal{H} . We thus have to find the domain $D(H) \subset \mathcal{H}$ corresponding to the situation depicted in Fig. 1 such that $H\psi \in \mathcal{H}$ for all $\psi \in D(H)$ and $\{H, D(H)\}$ is self-adjoint. The precise definition of a self-adjoint operator is given in Appendix A and we refer to the paper [20] for some physical motivations. This section is not crucial to understand the remainder of this paper, so the uninterested reader may look at the scattering matrix (7) and then go directly to the solution (19). In the paper [10], the scattering processes occurring at the connection point (between the loop and the lead) are described in terms of the following energy-independent (unitary) scattering matrix:

$$S = \begin{pmatrix} -(a+b) & \sqrt{\varepsilon} & \sqrt{\varepsilon} \\ \sqrt{\varepsilon} & a & b \\ \sqrt{\varepsilon} & b & a \end{pmatrix}, \quad (7)$$

where $a = \frac{1}{2}(\sqrt{1-2\varepsilon} - 1)$, $b = \frac{1}{2}(\sqrt{1-2\varepsilon} + 1)$, and $\varepsilon \in (0, \frac{1}{2}]$. Here, $\varepsilon = 0$ corresponds to the uncoupled situation (which is excluded) and $\varepsilon = \frac{1}{2}$ to the maximally coupled one. Note that a and b never vanish. To implement such a scattering matrix, it is convenient to work in the local reference coordinates $\{x_1 \in [0, \infty) \text{ and } x_2, x_3 \in [0, L]\}$ associated with

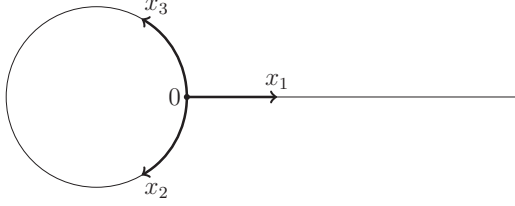


FIG. 2. The local reference coordinates.

the three branches exiting from the connection point $x_1 = x_2 = x_3 = 0$; see Fig. 2. Then, a general scattering matrix $S(k)$ at energy $k^2 > 0$, with $k > 0$, relates the incoming and outgoing amplitudes at the connection point through the following solutions of the stationary Schrödinger equation $H\varphi^\ell = k^2\varphi^\ell$, with $k > 0$ and $\ell = 1, 2, 3$:

$$\varphi_1^\ell(x_1) = \delta_{1\ell}e^{-ikx_1} + S_{1\ell}(k)e^{ikx_1}, \quad (8)$$

$$\varphi_2^\ell(x_2) = [\delta_{2\ell}e^{-ikx_2} + S_{2\ell}(k)e^{ikx_2}]e^{i\frac{\Phi}{L}x_2}, \quad (9)$$

$$\varphi_3^\ell(x_3) = [\delta_{3\ell}e^{-ikx_3} + S_{3\ell}(k)e^{ikx_3}]e^{-i\frac{\Phi}{L}x_3}, \quad (10)$$

where δ_{ij} is the Kronecker delta. Inspired from quantum networks studies [21–24], we shall now derive the corresponding boundary conditions at the connection point insuring the self-adjointness of the Hamiltonian H .

Let f and g be two functions in \mathcal{H} such that Hf and Hg are still in \mathcal{H} . Then, a simple calculation gives

$$\langle f | Hg \rangle = \langle Hf | g \rangle + \text{BT}, \quad (11)$$

where $\langle \cdot | \cdot \rangle$ denotes the usual scalar product in $L^2([0, \infty))$ and BT contains the boundary terms appearing during the integrations by parts:

$$\begin{aligned} \text{BT} = & \sum_{j=1}^3 [\overline{f_j(0)}g_j'(0) - \overline{f_j'(0)}g_j(0)] \\ & + 2i\frac{\Phi}{L}[\overline{f_3(0)}g_3(0) - \overline{f_2(0)}g_2(0)], \end{aligned} \quad (12)$$

where $f_1(x_1) = f(L + x_1)$, $f_2(x_2) = f(x_2)$, $f_3(x_3) = f(L - x_3)$, and similarly for g_1, g_2 , and g_3 . The self-adjointness of H requires that BT vanishes for all $\mathbf{f} = (f_1, f_2, f_3)$ and $\mathbf{g} = (g_1, g_2, g_3)$ satisfying the same boundary conditions at $x_1 = x_2 = x_3 = 0$ (see Appendix A for a more precise statement). Setting $\mathbf{f} = \mathbf{g}$, one thus has the following necessary condition:

$$\langle \mathbf{f}(0) | \mathbf{f}'(0) \rangle_{\mathbb{C}^3} - \langle \mathbf{f}'(0) | \mathbf{f}(0) \rangle_{\mathbb{C}^3} + 2i\frac{\Phi}{L}[|f_3(0)|^2 - |f_2(0)|^2] = 0, \quad (13)$$

where $\langle \cdot | \cdot \rangle_{\mathbb{C}^3}$ denotes the canonical scalar product in \mathbb{C}^3 . If $\|\cdot\|_{\mathbb{C}^3} = \sqrt{\langle \cdot | \cdot \rangle_{\mathbb{C}^3}}$, then (13) is satisfied if and only if $\|\mathbf{f}(0) + i[\mathbf{f}'(0) - i\frac{\Phi}{L}\mathbf{h}(0)]\|_{\mathbb{C}^3} = \|\mathbf{f}(0) - i[\mathbf{f}'(0) - i\frac{\Phi}{L}\mathbf{h}(0)]\|_{\mathbb{C}^3}$, where $\mathbf{h}(0) = (0, f_2(0), -f_3(0))$. This is the case if and only if there is a unitary matrix U such that

$$\mathbf{f}(0) + i\left[\mathbf{f}'(0) - i\frac{\Phi}{L}\mathbf{h}(0)\right] = U\left\{\mathbf{f}(0) - i\left[\mathbf{f}'(0) - i\frac{\Phi}{L}\mathbf{h}(0)\right]\right\}, \quad (14)$$

or

$$(\mathbb{1} - U)\mathbf{f}(0) + i(\mathbb{1} + U)\left[\mathbf{f}'(0) - i\frac{\Phi}{L}\mathbf{h}(0)\right] = 0. \quad (15)$$

We thus have the following necessary condition for the self-adjointness of $\{H, D(H)\}$: There must be a unitary matrix U such that the boundary conditions (15) are satisfied for all $f \in D(H)$.

To specify the boundary conditions (15) in terms of the scattering matrix $S(k)$, one requires that the scattering states φ^ℓ (which are not in \mathcal{H}) satisfy the relation (15). Setting $f = \varphi^\ell$, with $\ell = 1, 2$, or 3 , one easily checks that the relation (15) is verified with $U = [(k + 1)S(k) - (k - 1)\mathbb{1}] \times [(k + 1)\mathbb{1} - (k - 1)S(k)]^{-1}$, which means that the scattering matrix may be written as $S(k) = [(k - 1)\mathbb{1} + (k + 1)U] \times [(k + 1)\mathbb{1} + (k - 1)U]^{-1}$. Note that the knowledge of the scattering matrix $S(k)$ at any energy $E = k^2$ uniquely determines the boundary conditions (15) and that if S does not depend on k , then one simply has $U = S$. Returning to our original reference frame, the scattering matrix (7) leads to the following boundary conditions:

$$\psi(0_+) - \psi(L_-) = 0, \quad (16)$$

$$\sqrt{\varepsilon}\psi(0_+) - b\psi(L_+) = 0, \quad (17)$$

$$\sqrt{\varepsilon}\psi'(L_+) + b[\psi'(0_+) - \psi'(L_-)] = 0. \quad (18)$$

Note that these conditions do not depend on the magnetic flux Φ , that they are contained in the model considered in [16], and that the free boundary conditions $\psi(0_+) = \psi(L_-) = \psi(L_+)$ and $\psi'(L_-) = \psi'(0_+) + \psi'(L_+)$ correspond to the case $\varepsilon = 4/9$. As explained previously, the boundary conditions (16)–(18) are necessary for H to be self-adjoint. In Appendix A, we show that these boundary conditions are also sufficient for H to be self-adjoint. Therefore, we deduce that the relations (16)–(18) are in fact the unique boundary conditions associated with the scattering matrix (7) for which the Hamiltonian (6) is self-adjoint. More precisely, the Hamiltonian H associated with S is self-adjoint if and only if

$$D(H) = \{\psi \in \mathcal{H} \mid H\psi \in \mathcal{H} \text{ and (16)–(18) are satisfied}\}. \quad (19)$$

III. THE PROPAGATOR

Let us recall that the model we are describing contains three parameters: the loop’s length $L > 0$, the magnetic flux $\Phi \in \mathbb{R}$, and the coupling parameter $\varepsilon \in (0, \frac{1}{2}]$. In what follows, we shall suppose that their values are kept constant and that at time $t = 0$ the initial state $\psi_0 \in D(H)$ of the particle is localized in the loop [i.e., it satisfies $\psi_0(x) = 0$, for all $x \notin [0, L]$], and is normalized: $\int_0^L |\psi_0(x)|^2 dx = 1$. Note that the property $\psi_0(L_+) = \psi_0'(L_+) = 0$ together with the boundary conditions (16)–(18) imply $\psi_0(0_+) = \psi_0(L_-) = 0$ and $\psi_0'(0_+) = \psi_0'(L_-)$. Then, the nonescape probability is given by ($t > 0$)

$$P(\psi_0, L, \Phi, \varepsilon, t) = \int_0^L |\psi(x, t)|^2 dx, \quad (20)$$

where the wave function obeys the Schrödinger equation,

$$i\frac{\partial}{\partial t}\psi(x, t) = H\psi(x, t), \quad \text{with} \quad \psi(x, 0) = \psi_0(x). \quad (21)$$

We see that we need to solve the Schrödinger equation (21) inside the loop ($x \in [0, L]$) in order to compute the nonescape probability (20). To determine $\psi(x, t)$ we shall write the initial state $\psi_0(x)$ as a superposition of generalized eigenstates of H , satisfying (16)–(18), over the spectrum of H , which is $\sigma(H) = [0, \infty)$ (see Appendix A).

Let $k > 0$, then the general solution of the time-independent Schrödinger equation $H\varphi_k = k^2\varphi_k$ is

$$\varphi_k(x) = [A(k)e^{ikx} + B(k)e^{-ikx}]e^{i\frac{\Phi}{L}x}\chi_{[0,L)}(x) + [C(k)e^{ik(x-L)} + D(k)e^{-ik(x-L)}]\chi_{[L,\infty)}(x), \quad (22)$$

where $A(k)$, $B(k)$, $C(k)$, and $D(k)$ are complex numbers. We shall choose these constants such that the boundary conditions (16)–(18) are satisfied and such that the generalized eigenstates $\{\varphi_k(x)\}$ are δ normalized [as we shall see $\varphi_{-k}(x) = -\varphi_k(x)$, so only the $\varphi_k(x)$ with positive k needs to be considered]:

$$\langle \varphi_k | \varphi_p \rangle = \int_0^\infty \overline{\varphi_k(x)} \varphi_p(x) dx = \delta(k - p), \quad \text{for all } k, p > 0. \quad (23)$$

Solving (16)–(18) and (23), one finds [25]

$$A(k) = \frac{e^{-i(kL-\Phi)} - 1}{\Omega(k)}, \quad (24)$$

$$B(k) = -\frac{e^{i(kL+\Phi)} - 1}{\Omega(k)}, \quad (25)$$

$$C(k) = \frac{1}{2b\sqrt{\varepsilon}} \frac{(2b - \varepsilon)(1 + e^{2i\Phi}) - 2(b - \varepsilon)e^{-i(kL-\Phi)} - 2be^{i(kL+\Phi)}}{\Omega(k)}, \quad (26)$$

$$D(k) = -\frac{1}{2b\sqrt{\varepsilon}} \frac{(2b - \varepsilon)(1 + e^{2i\Phi}) - 2(b - \varepsilon)e^{i(kL+\Phi)} - 2be^{-i(kL-\Phi)}}{\Omega(k)}, \quad (27)$$

where

$$\Omega(k) = \left\{ \frac{8\pi}{\varepsilon} [a^2 \sin^2(kL) + b^2 [\cos(kL) - \cos(\Phi)]^2] \right\}^{1/2}. \quad (28)$$

In Appendix B, we show that the coefficients A , B , C , and D are well defined in \mathbb{R} . In addition, if $\cos(\Phi) = 1$ or $\cos(\Phi) = -1$, there are the bound states $\tilde{\varphi}_n^+, \tilde{\varphi}_n^- \in D(H)$ of H ($C = D = 0$ and $A = -B$):

$$\cos(\Phi) = 1 : \tilde{\varphi}_n^+(x) = \sqrt{\frac{2}{L}} \sin(k_{2n}x) e^{i\frac{\Phi}{L}x} \chi_{[0,L)}(x), \quad (29)$$

$$n = 1, 2, \dots,$$

$$\cos(\Phi) = -1 : \tilde{\varphi}_n^-(x) = \sqrt{\frac{2}{L}} \sin(k_{2n+1}x) e^{i\frac{\Phi}{L}x} \chi_{[0,L)}(x), \quad (30)$$

$$n = 0, 1, \dots,$$

where $k_n = \frac{n\pi}{L}$. Note that the eigenvalues $E_n = \left(\frac{n\pi}{L}\right)^2$, with $n = 1, 2, \dots$, associated with the bound states (29)–(30) are as expected inside the continuous spectrum $[0, \infty)$ of H . If $\cos(\Phi) = 1$, then one has for all $m, n = 1, 2, \dots$, and every $k > 0$ ($k \in \{\frac{2n\pi}{L}\}_{n=1}^\infty$ included):

$$\langle \tilde{\varphi}_m^+ | \tilde{\varphi}_n^+ \rangle = \delta_{mn} \quad \text{and} \quad \langle \varphi_k | \tilde{\varphi}_n^+ \rangle = 0. \quad (31)$$

Similarly, if $\cos(\Phi) = -1$, then for all $m, n = 0, 1, \dots$, and $k > 0$ ($k \in \{\frac{(2n+1)\pi}{L}\}_{n=0}^\infty$ included):

$$\langle \tilde{\varphi}_m^- | \tilde{\varphi}_n^- \rangle = \delta_{mn} \quad \text{and} \quad \langle \varphi_k | \tilde{\varphi}_n^- \rangle = 0. \quad (32)$$

Since the Hamiltonian H is self-adjoint, it follows from the spectral theorem that the family of states $\{\varphi_k, \delta_{\cos(\Phi), 1} \tilde{\varphi}_n^+, \delta_{\cos(\Phi), -1} \tilde{\varphi}_n^-\}$ generates the whole Hilbert

space \mathcal{H} . To avoid technical complications, we shall assume that the initial state ψ_0 can be written *punctually* in terms of these states [this assumption may be checked explicitly in the cases ($\varepsilon = 1/2, \Phi = 0$) and ($\varepsilon = 1/2, \Phi = \pi/2$)].

Assumption (completeness). Let $\psi_0 \in D(H)$ be an initial state localized in the loop. Then, we assume that for (almost) every $x \in [0, \infty)$,

$$\psi_0(x) = \int_0^\infty \langle \varphi_k | \psi_0 \rangle \varphi_k(x) dk + \delta_{\cos(\Phi), 1} \sum_{n=1}^\infty \langle \tilde{\varphi}_n^+ | \psi_0 \rangle \tilde{\varphi}_n^+(x) + \delta_{\cos(\Phi), -1} \sum_{n=0}^\infty \langle \tilde{\varphi}_n^- | \psi_0 \rangle \tilde{\varphi}_n^-(x). \quad (33)$$

Under this assumption and using the orthogonality relations (23) and (31)–(32), one may write the solution of the Schrödinger equation (21) as

$$\psi(x, t) = (e^{-iHt} \psi_0)(x) = \int_0^L K(x, y, t) \psi_0(y) dy, \quad (34)$$

where the propagator is

$$K(x, y, t) = \int_0^\infty e^{-ik^2 t} \varphi_k(x) \overline{\varphi_k(y)} dk + \delta_{\cos(\Phi), 1} \sum_{n=1}^\infty e^{-ik_{2n}^2 t} \tilde{\varphi}_n^+(x) \overline{\tilde{\varphi}_n^+(y)} + \delta_{\cos(\Phi), -1} \sum_{n=0}^\infty e^{-ik_{2n+1}^2 t} \tilde{\varphi}_n^-(x) \overline{\tilde{\varphi}_n^-(y)}. \quad (35)$$

Looking back at (20) and (34) one sees that it is sufficient to know the propagator $K(x, y, t)$ for $x, y \in [0, L]$. In this case, one may write

$$K(x, y, t) = K_1(x, y, t) + \delta_{\cos(\Phi), 1} K_2(x, y, t) + \delta_{\cos(\Phi), -1} K_3(x, y, t), \quad (36)$$

where

$$K_1(x, y, t) = e^{i\frac{\Phi}{L}(x-y)} \int_{-\infty}^{\infty} \{f_1(k)e^{-i(k^2t-k(x-y))} + f_2(k)e^{-i(k^2t-k(x+y))}\} dk, \quad (37)$$

$$K_2(x, y, t) = \frac{e^{i\frac{\Phi}{L}(x-y)}}{2L} \sum_{n=-\infty}^{\infty} \{e^{-i[k_{2n}^2t-k_{2n}(x-y)]} - e^{-i[k_{2n}^2t-k_{2n}(x+y)]}\}, \quad (38)$$

$$K_3(x, y, t) = \frac{e^{i\frac{\Phi}{L}(x-y)}}{2L} \sum_{n=-\infty}^{\infty} \{e^{-i[k_{2n+1}^2t-k_{2n+1}(x-y)]} - e^{-i[k_{2n+1}^2t-k_{2n+1}(x+y)]}\}, \quad (39)$$

with

$$k_n = \frac{n\pi}{L}, \quad n \in \mathbb{Z}, \quad (40)$$

$$f_1(k) = \frac{\varepsilon[1 - \cos(kL - \Phi)]}{4\pi\{a^2 \sin^2(kL) + b^2[\cos(kL) - \cos(\Phi)]^2\}}, \quad (41)$$

$$f_2(k) = -\frac{\varepsilon[1 + e^{-2ikL} - 2e^{-ikL} \cos(\Phi)]}{8\pi\{a^2 \sin^2(kL) + b^2[\cos(kL) - \cos(\Phi)]^2\}}. \quad (42)$$

Clearly, the propagator $K_1(x, y, t)$ describes the decaying aspect of the initial state ψ_0 , while the two other propagators, $K_2(x, y, t)$ and $K_3(x, y, t)$, describe the stationary aspect of ψ_0 , (i.e., the part of ψ_0 which remains in the loop for all times [26]).

In the case ($\varepsilon = 1/2, \Phi = \pi/2$), one has $\Omega(k) = \sqrt{4\pi}$ and one may evaluate the propagator exactly by splitting the different terms. We find

$$K(x, y, t) = \frac{e^{i\frac{\pi}{2L}(x-y)}}{\sqrt{16\pi it}} \left[2e^{i\frac{(x-y)^2}{4t}} - e^{i\frac{(x+y)^2}{4t}} - e^{i\frac{(x+y-2L)^2}{4t}} + ie^{i\frac{(x-y+L)^2}{4t}} - ie^{i\frac{(x-y-L)^2}{4t}} \right]. \quad (43)$$

Also, in the case ($\varepsilon = 1/2, \Phi = 0$), one has $f_1(k) = 1/(4\pi)$ and $f_2(k) = e^{-ikL}/(4\pi)$, so that

$$K(x, y, t) = \frac{1}{\sqrt{16\pi it}} \left[e^{i\frac{(x-y)^2}{4t}} + e^{i\frac{(x+y-L)^2}{4t}} \right] + K_2(x, y, t). \quad (44)$$

In general, we are not able to integrate explicitly $K_1(x, y, t)$, so we shall only discuss its long time behavior [some comments concerning the short-time behavior of $P(\psi_0, L, \Phi, \varepsilon, t)$ can be found in Sec. VIII]. For this, we need to analyze the asymptotic behavior of an integral of the following form:

$$I(t) = \int_{-\infty}^{\infty} f(k)e^{-i(k^2t-kz)} dk, \quad (45)$$

where f is either f_1 or f_2 and $z = (x \pm y) \in \mathbb{R}$. Looking at the expressions (41)-(42), (B5)-(B6) and (B8)-(B9), it is clear

that, for any $k \in \mathbb{R}$, the function $f(k)$ may be written as a Maclaurin series:

$$f(k) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} k^n. \quad (46)$$

Substituting this expression in (45) and exchanging formally the order of integration and summation we obtain

$$I(t) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \int_{-\infty}^{\infty} k^n e^{-i(k^2t-kz)} dk. \quad (47)$$

We next use the following identity (see Appendix C):

$$\int_{-\infty}^{\infty} k^n e^{-ak^2+bk} dk = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}} \sum_{\ell=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{\ell! (n-2\ell)!} \frac{(2b)^{n-2\ell}}{(4a)^{n-\ell}}, \quad (48)$$

where $\lfloor \frac{n}{2} \rfloor = n/2$ if n is even and $(n-1)/2$ if n is odd, and $a, b \in \mathbb{C} \setminus \{0\}$, with $\text{Re}(a) > 0$. The cases $b = 0$ and $\text{Re}(a) = 0$ are obtained as the limiting expressions of the right-hand side of (48) as $b \rightarrow 0$ and $\text{Re}(a) \rightarrow 0^+$, respectively. Thus, writing

$$e^{i\frac{z^2}{4t}} = \sum_{m=0}^{\infty} \frac{1}{m!} \frac{i^m z^{2m}}{(4t)^m}, \quad (49)$$

we obtain

$$I(t) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \sum_{\ell=0}^{\lfloor \frac{n}{2} \rfloor} \frac{\sqrt{\pi} i^{m-\ell-1/2}}{2^{2m+n} m! \ell! (n-2\ell)!} f^{(n)}(0) z^{2(m-\ell)+n} \times \frac{1}{t^{[2(m+n-\ell)+1]/2}}. \quad (50)$$

Using the relation (50), one can write

$$K_1(x, y, t) = e^{i\frac{\Phi}{L}(x-y)} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \sum_{\ell=0}^{\lfloor \frac{n}{2} \rfloor} \frac{\sqrt{\pi} i^{m-\ell-1/2}}{2^{2m+n} m! \ell! (n-2\ell)!} \times \frac{1}{t^{[2(m+n-\ell)+1]/2}} \left[f_1^{(n)}(0) (x-y)^{2(m-\ell)+n} + f_2^{(n)}(0) (x+y)^{2(m-\ell)+n} \right], \quad (51)$$

where the functions f_1 and f_2 are given by (41)-(42). The first two leading terms are

$$K_1(x, y, t) = e^{i\frac{\Phi}{L}(x-y)} \left\{ \sqrt{\frac{\pi}{i}} [f_1(0) + f_2(0)] \frac{1}{t^{1/2}} + \left\{ \frac{\sqrt{\pi} i}{4} [f_1(0)(x-y)^2 + f_2(0)(x+y)^2] + \sqrt{\frac{\pi}{4i}} [f_1'(0)(x-y) + f_2'(0)(x+y)] + \frac{\sqrt{\pi}}{4i^{3/2}} [f_1''(0) + f_2''(0)] \right\} \frac{1}{t^{3/2}} \right\} + O\left(\frac{1}{t^{5/2}}\right). \quad (52)$$

A careful analysis of the expressions (41)-(42) shows that one has to deal with two cases (see also Appendix B): $\cos(\Phi) = 1$ and $\cos(\Phi) \neq 1$. In particular, one has

$$f_1(0) = f_2(0) = \frac{\varepsilon}{8\pi a^2} \quad \text{if } \cos(\Phi) = 1, \quad (53)$$

$$f_1(0) = -f_2(0) = \frac{\varepsilon}{4\pi b^2[1 - \cos(\Phi)]} \quad \text{if } \cos(\Phi) \neq 1. \quad (54)$$

As we shall see, the fact that $f_1(0) = f_2(0)$ in the first case, while $f_1(0) = -f_2(0)$ in the second, will lead to a drastic

change in the decay properties of the nonescape probability.

If $\cos(\Phi) = 1$, then

$$\begin{aligned} K(x, y, t) &= K_2(x, y, t) + \frac{\varepsilon e^{i\frac{\Phi}{L}(x-y)}}{\sqrt{16\pi i} a^2} \left\{ \frac{1}{t^{1/2}} + \frac{i}{4} [x^2 + y^2] \right. \\ &\quad \left. - L(x+y) + \frac{L^2}{2} \left(\frac{b}{a}\right)^2 \frac{1}{t^{3/2}} \right\} + O\left(\frac{1}{t^{5/2}}\right). \end{aligned} \quad (55)$$

If $\cos(\Phi) \neq 1$, then

$$\begin{aligned} K(x, y, t) &= \delta_{\cos(\Phi), -1} K_3(x, y, t) - \frac{i\varepsilon e^{i\frac{\Phi}{L}(x-y)}}{8\sqrt{\pi i} b^2} \\ &\quad \times \frac{\{L - [1 - \cos(\Phi) + i \sin(\Phi)]x\} \{L - [1 - \cos(\Phi) - i \sin(\Phi)]y\}}{[1 - \cos(\Phi)]^2} \frac{1}{t^{3/2}} + O\left(\frac{1}{t^{5/2}}\right). \end{aligned} \quad (56)$$

As one may easily check, the expression (55) with $(\varepsilon = 1/2, \Phi = 0)$ and the expression (56) with $(\varepsilon = 1/2, \Phi = \pi/2)$ coincide with the leading terms of (44) and (43), respectively.

IV. GENERAL RESULTS

From the relations (55)-(56), it follows that

$$\lim_{t \rightarrow \infty} P(\psi_0, L, \Phi, \varepsilon, t) = \begin{cases} P_\infty(\psi_0, L, \Phi) & \text{if } |\cos(\Phi)| = 1 \\ 0 & \text{otherwise} \end{cases}, \quad (57)$$

where

$$\begin{aligned} P_\infty(\psi_0, L, \Phi) &= \int_0^L dx \left| \int_0^L dy [\delta_{\cos(\Phi), 1} K_2(x, y, 0) \right. \\ &\quad \left. + \delta_{\cos(\Phi), -1} K_3(x, y, 0)] \psi_0(y) \right|^2. \end{aligned} \quad (58)$$

If $\cos(\Phi) = 1$ [or $\cos(\Phi) = -1$], then the initial state ψ_0 may be written as a sum of two terms [see (33)], one associated with the scattering states φ_k and the other with the bound states $\tilde{\varphi}_n^+$ [or $\tilde{\varphi}_n^-$]. The part associated with the bound states will lead to a nonzero value of $P_\infty(\psi_0, L, \Phi)$. Note that $P_\infty(\psi_0, L, \Phi)$ does not depend on ε . From the expressions (55)-(56), one sees that the large-time behavior of $P(\psi_0, L, \Phi, \varepsilon, t)$ depends drastically on the value of $\cos(\Phi)$. Nevertheless, setting $P_\infty(\psi_0, L, \Phi) = 0$ whenever $|\cos(\Phi)| \neq 1$, one may write

$$P(\psi_0, L, \Phi, \varepsilon, t) = P_\infty(\psi_0, L, \Phi) + \sum_{k=1}^{\infty} \frac{C_k(\psi_0, L, \Phi, \varepsilon)}{t^k}. \quad (59)$$

To obtain explicit expressions for the coefficients $C_k(\psi_0, L, \Phi, \varepsilon)$, it is convenient to write the expression (51) in the following form:

$$K_1(x, y, t) = \sum_{\ell=0}^{\infty} \frac{G_\ell(x, y)}{t^{(2\ell+1)/2}}. \quad (60)$$

Then, the decaying part of the wave function reads

$$\psi_{\text{decay}}(x, t) \equiv \int_0^L K_1(x, y, t) \psi_0(y) dy = \sum_{\ell=0}^{\infty} \frac{Q_\ell(x)}{t^{(2\ell+1)/2}}, \quad (61)$$

where

$$Q_\ell(x) = \int_0^L G_\ell(x, y) \psi_0(y) dy. \quad (62)$$

Hence,

$$\begin{aligned} P(\psi_0, L, \Phi, \varepsilon, t) - P_\infty(\psi_0, L, \Phi) &= \int_0^L |\psi_{\text{decay}}(x, t)|^2 dx = \sum_{k=1}^{\infty} \frac{C_k(\psi_0, L, \Phi, \varepsilon)}{t^k}, \end{aligned} \quad (63)$$

where

$$C_k(\psi_0, L, \Phi, \varepsilon) = \sum_{\substack{\ell, m=0 \\ \ell+m+1=k}}^{\infty} \langle Q_m | Q_\ell \rangle. \quad (64)$$

Note that if $C_1(\psi_0, L, \Phi, \varepsilon) = 0$, then $Q_0 \equiv 0$ and thus $C_2(\psi_0, L, \Phi, \varepsilon) = 0$. More generally, if $C_1(\psi_0, L, \Phi, \varepsilon) = C_2(\psi_0, L, \Phi, \varepsilon) = \dots = C_{2\ell+1}(\psi_0, L, \Phi, \varepsilon) = 0$, then $C_{2\ell+2}(\psi_0, L, \Phi, \varepsilon) = 0$. Thus, at large times the nonescape probability $P(\psi_0, L, \Phi, \varepsilon, t) \sim C_\delta(\psi_0, L, \Phi, \varepsilon)/t^\delta$, with δ an odd number. Let us use the expressions (55)-(56) to write the leading coefficients $C_k(\psi_0, L, \Phi, \varepsilon)$. It turns out that they can be nicely written in terms of the derivatives of the Fourier transform of the initial state:

$$\tilde{\psi}_0^{(n)}(k) = \frac{(-i)^n}{\sqrt{2\pi}} \int_0^L e^{-iky} y^n \psi_0(y) dy. \quad (65)$$

There are two cases:

(1) If $\cos(\Phi) = 1$, then

$$C_1(\psi_0, L, \Phi, \varepsilon) = \frac{\varepsilon^2 L}{8 a^4} \left| \tilde{\psi}_0 \left(\frac{\Phi}{L} \right) \right|^2. \quad (66)$$

If $C_1(\psi_0, L, \Phi, \varepsilon) = 0$, then $C_2(\psi_0, L, \Phi, \varepsilon) = 0$ and the next leading term is given by

$$C_3(\psi_0, L, \Phi, \varepsilon) = \frac{\varepsilon^2 L}{128 a^4} \left| L \tilde{\psi}'_0 \left(\frac{\Phi}{L} \right) - i \tilde{\psi}''_0 \left(\frac{\Phi}{L} \right) \right|^2. \quad (67)$$

(2) If $\cos(\Phi) \neq 1$, then $C_1(\psi_0, L, \Phi, \varepsilon) = C_2(\psi_0, L, \Phi, \varepsilon) = 0$ and

$$\begin{aligned} C_3(\psi_0, L, \Phi, \varepsilon) &= \frac{\varepsilon^2 L^3 [2 + \cos(\Phi)]}{96 b^4 [1 - \cos(\Phi)]^4} \left| L \tilde{\psi}'_0 \left(\frac{\Phi}{L} \right) \right. \\ &\quad \left. - [\sin(\Phi) + i[1 - \cos(\Phi)]] \tilde{\psi}'_0 \left(\frac{\Phi}{L} \right) \right|^2. \quad (68) \end{aligned}$$

ψ_0 dependence. We see that only the momentum $k = \Phi/L$ plays a role in the decaying properties of $P(\psi_0, L, \Phi, \varepsilon, t)$. When $\Phi = 0$, this coincides with the well-known fact that only the zero momentum is involved [3]. Note that $C_1(\psi_0, L, \Phi, \varepsilon) \neq 0$ only if $\cos(\Phi) = 1$ and $\tilde{\psi}'_0(\Phi/L) \neq 0$. As an illustration, let us discuss the case $\Phi = 0$. In this case, the bound states (29) form a basis in $L^2([0, L])$ of all odd functions with respect to $L/2$ [i.e., $\psi(x) = -\psi(L-x)$ for all $x \in [0, L]$]. Thus, if $\Phi = 0$ and the initial state $\psi_0 \in D(H)$ is an odd function with respect to $L/2$, then $P(\psi_0, L, \Phi, \varepsilon, t) = P_\infty(\psi_0, L, \Phi) = 1$ for all times. On the contrary, if $\Phi = 0$ and $\psi_0 \in D(H)$ is an even function with respect to $L/2$ [i.e., $\psi_0(x) = \psi_0(L-x)$ for all $x \in [0, L]$], then $P_\infty(\psi_0, L, \Phi) = 0$ and $P(\psi_0, L, \Phi, \varepsilon, t) = C_1(\psi_0, L, \Phi, \varepsilon)/t + O(1/t^2)$ at large times, with $C_1(\psi_0, L, \Phi, \varepsilon) \neq 0$ since $\int_0^L \psi_0(y) dy \neq 0$. More generally, if $\Phi = 0$ and $\psi_0 = \psi_0^{\text{odd}} + \psi_0^{\text{even}}$, then $P(\psi_0, L, \Phi, \varepsilon, t) = P_\infty(\psi_0, L, \Phi) + C_1(\psi_0, L, \Phi, \varepsilon)/t + O(1/t^2)$, where $P_\infty(\psi_0, L, \Phi) = \int_0^L dx \left| \int_0^L dy K_2(x, y, 0) \psi_0^{\text{odd}}(y) \right|^2$ and $C_1(\psi_0, L, \Phi, \varepsilon) = \varepsilon^2 L / (8a^4) \left| \tilde{\psi}'_0^{\text{even}}(0) \right|^2$.

L dependence. Let $\psi_0(x, \lambda)$ and $K(x, y, t, \lambda)$ be the initial state and the propagator corresponding to a loop of length λL , with $\lambda > 0$. Then, from the relations (72) and (36), one deduces that

$$\sqrt{\lambda} \psi_0(\lambda x, \lambda) = \psi_0(x, 1), \quad (69)$$

$$\lambda K(\lambda x, \lambda y, \lambda^2 t, \lambda) = K(x, y, t, 1). \quad (70)$$

From these scaling laws, one finds that

$$P(\psi_0, \lambda L, \Phi, \varepsilon, t) = P \left(\psi_0, L, \Phi, \varepsilon, \frac{t}{\lambda^2} \right). \quad (71)$$

From the relation (59), one easily deduces that P_∞ is independent of L , so from now on we shall write $P_\infty(\psi_0, \Phi)$, and that the coefficient C_k is an homogeneous function of degree $2k$ [i.e., $C_k(\psi_0, \lambda L, \Phi, \varepsilon) = \lambda^{2k} C_k(\psi_0, L, \Phi, \varepsilon)$ for all $\lambda > 0$], and thus $C_k(\psi_0, L, \Phi, \varepsilon) \propto L^{2k}$.

Φ dependence. Looking at the relations (66)–(68), one sees that in general it is difficult to predict the Φ dependence of $P(\psi_0, L, \Phi, \varepsilon, t)$ and we shall discuss this matter in detail in the next section. Nevertheless, some general symmetries can be found. Indeed, the propagators $K_j(x, y, t)$, with $j = 1, 2, 3$, become $e^{i \frac{2\pi}{L}(x-y)} K_j(x, y, t)$ under the transformation $\Phi \mapsto \Phi + 2\pi$. This implies that $P(\psi_0, L, \Phi, \varepsilon, t)$ is invariant under this transformation on the proviso that one replaces

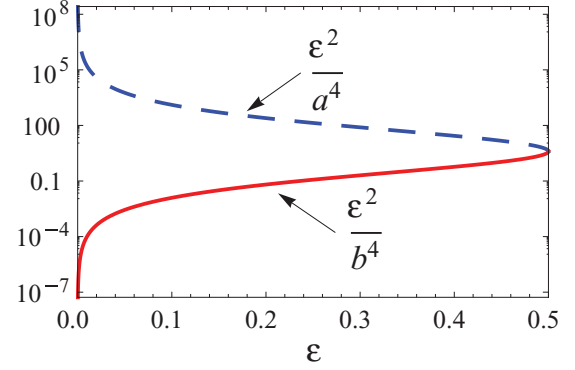


FIG. 3. (Color online) Log-lin plot of ε^2/a^4 (dashed blue) and ε^2/b^4 (red) for $\varepsilon \in [0, 0.5]$.

the initial state $\psi_0(y)$ by $e^{-i \frac{2\pi}{L} y} \psi_0(y)$. Furthermore, a simple calculation shows that $P(\psi_0, L, \Phi, \varepsilon, t)$ is invariant under the transformation $\Phi \mapsto -\Phi$ if the initial state satisfies $\psi_0(x) = -\psi_0(L-x)$ [as in (72)] or $\psi_0(x) = \psi_0(L-x)$, for all $x \in [0, L]$.

ε dependence. At large times, one sees from (66)–(68) that $P(\psi_0, L, \Phi, \varepsilon, t) - P_\infty(\psi_0, \Phi)$ behaves as ε^2/a^4 if $\cos(\Phi) = 1$ and ε^2/b^4 otherwise. Looking at Fig. 3, one deduces that at large times $P(\psi_0, L, \Phi, \varepsilon, t) - P_\infty(\psi_0, \Phi)$ decreases with ε if $\cos(\Phi) = 1$ and increases otherwise. In other words, in the long run the particle escapes faster as one increases ε if $\cos(\Phi) = 1$ and escapes slower otherwise. This slowing effect when $\cos(\Phi) \neq 1$ at large times is rather peculiar since in the short time regime, some numerical results show (see Fig. 10) that the particle may escape faster as ε increases.

V. THE BOUND STATES

In order to apply our general results, let us consider the following situation: The system is prepared such that at time $t = 0$ no magnetic flux crosses the loop and the particle is in a bound state $\varphi_n \in D(H)$, where

$$\varphi_n(x) = \sqrt{\frac{2}{L}} \sin \left(\frac{2\pi n}{L} x \right) \chi_{[0, L]}(x), \quad n = 1, 2, \dots \quad (72)$$

Since the effect of the length's loop and of the coupling parameter was thoroughly discussed in Sec. IV, let us fix L and ε and discuss the Φ dependence of $P(\varphi_n, L, \Phi, \varepsilon, t)$. If at all later times there is still no magnetic flux inside the loop ($\Phi = 0$), then all the bound states φ_n will lead naturally to $P(\varphi_n, L, \Phi, \varepsilon, t) = 1$ at all times (i.e., the particle will remain forever in the loop). On the contrary, if some constant magnetic field is applied ($\Phi \neq 0$), then the states φ_n will no longer be bound states of the Hamiltonian and consequently the particle may escape from the loop. Using (58), one finds the following asymptotic values:

$$\begin{aligned} \lim_{t \rightarrow \infty} P(\varphi_n, L, \Phi, \varepsilon, t) &= P_\infty(\varphi_n, \Phi) \\ &= \begin{cases} 1 & \text{if } \Phi = 0 \\ 0 & \text{if } |\cos(\Phi)| \neq 1 \\ 1/4 & \text{if } |\Phi| = 2n\pi \\ 1/2 & \text{otherwise} \end{cases}. \quad (73) \end{aligned}$$

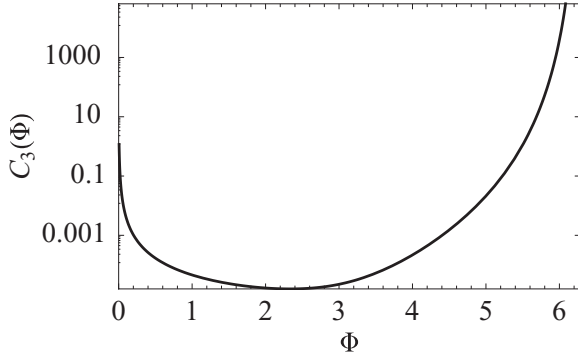


FIG. 4. Log-lin plot of $C_3(\varphi_n, L, \Phi, \varepsilon)$ in (74) as a function of flux $\Phi \in (0, 2\pi)$ for $n = 1$, $L = 1$, and $\varepsilon = 1/2$.

As explained in Sec. IV, $P(\varphi_n, L, \Phi, \varepsilon, t)$ is invariant under $\Phi \mapsto -\Phi$ since φ_n are odd functions with respect to $L/2$, so it is sufficient to discuss the case $\Phi \geq 0$. If $\Phi = 0$, then $P(\varphi_n, L, \Phi, \varepsilon, t) = 1$ at all times. If $\Phi \in (0, 2\pi)$, then by using (73) and (68) one finds $P(\varphi_n, L, \Phi, \varepsilon, t) = \delta_{\Phi, \pi}/2 + C_3(\varphi_n, L, \Phi, \varepsilon)/t^3 + O(1/t^4)$, where

$$C_3(\varphi_n, L, \Phi, \varepsilon) = \frac{2n^2\varepsilon^2\Phi^2L^6\pi[2 + \cos(\Phi)]}{3b^4[1 - \cos(\Phi)]^2(\Phi - 2n\pi)^4(\Phi + 2n\pi)^4}. \quad (74)$$

A simple analysis of (74) reveals that $C_3(\varphi_n, L, \Phi, \varepsilon)$ is always positive and diverges at the excluded values $\cos(\Phi) = 1$. Furthermore, we see in Fig. 4 that $C_3(\varphi_n, L, \Phi, \varepsilon)$ first decreases and then increases with Φ . Note also that $C_3(\varphi_n, L, \Phi, \varepsilon)$ decreases with n , showing that in the long run more energetic bound states escape faster from the loop. If $\Phi = 2\pi$ or more generally if $\cos(\Phi) = 1$, then by using (66)-(67) one finds $P(\varphi_n, L, \Phi, \varepsilon, t) = P_\infty(\varphi_n, \Phi) + C_1(\varphi_n, L, \Phi, \varepsilon)/t + C_2(\varphi_n, L, \Phi, \varepsilon)/t^2 + C_3(\varphi_n, L, \Phi, \varepsilon)/t^3 + O(1/t^4)$, where

$$C_1(\varphi_n, L, \Phi, \varepsilon) = \begin{cases} L^2\varepsilon^2/(32\pi a^4) & \text{if } |\Phi| = 2n\pi \\ 0 & \text{otherwise} \end{cases}. \quad (75)$$

If $C_1(\varphi_n, L, \Phi, \varepsilon) = 0$ (i.e., $|\Phi| \neq 2n\pi$), then $C_2(\varphi_n, L, \Phi, \varepsilon) = 0$ and

$$C_3(\varphi_n, L, \Phi, \varepsilon) = \frac{n^2\varepsilon^2\Phi^2L^6\pi}{2a^4(\Phi - 2n\pi)^4(\Phi + 2n\pi)^4}. \quad (76)$$

Note that, as in (74), the coefficient $C_3(\varphi_n, L, \Phi, \varepsilon)$ in (76) decreases with n . Note also that $C_3(\varphi_n, L, \Phi, \varepsilon)$ decreases with Φ , as one may easily see by looking at the red dots in Fig. 5. Finally, we see in Fig. 5 that by increasing further the magnetic flux Φ we obtain a series of similar patterns in each range $[2\ell\pi, 2(\ell + 1)\pi]$, $\ell = 0, 1, 2, \dots$

To obtain a global picture in time, we have computed $P(\varphi_n, L, \Phi, \varepsilon, t)$ numerically. For this, we wrote (37) as

$$K_1(x, y, t) = \int_{-\infty}^{\infty} G(k; x, y, t) dk = 2 \int_0^{\infty} G^s(k; x, y, t) dk, \quad (77)$$

where

$$G^s(k; x, y, t) = \frac{1}{2}[G(k; x, y, t) + G(-k; x, y, t)], \quad (78)$$

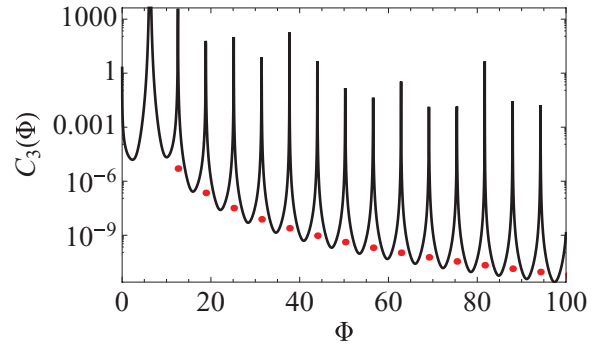


FIG. 5. (Color online) Log-lin plot of $C_3(\varphi_n, L, \Phi, \varepsilon)$ as a function of flux $\Phi \in [0, 100]$ for $n = 1$, $L = 1$, and $\varepsilon = 1/2$. When $\Phi = 0$, $C_3(\varphi_{n=1}, L = 1, \Phi, \varepsilon = 1/2) = 0$. When $\Phi = 2\pi$, $C_1(\varphi_{n=1}, L = 1, \Phi, \varepsilon = 1/2) \neq 0$ so $C_3(\varphi_{n=1}, L = 1, \Phi, \varepsilon = 1/2)$ is not plotted. When $\Phi = 4\pi, 6\pi, \dots$, we use (76) to obtain the red dots. All the other values are obtained with (74).

so that

$$P(\varphi_n, L, \Phi, \varepsilon, t) = 4 \int_0^{\infty} \int_0^{\infty} \left[\int_0^L \int_0^L \int_0^L G^s(k; x, y, t) \times \overline{G^s(p; x, z, t)} \overline{\psi_0(y)} \overline{\psi_0(z)} dx dy dz \right] dk dp. \quad (79)$$

Then, we integrated analytically the expression inside the square brackets and then computed numerically (with Matlab) the so obtained expression with respect to k and p over the finite domain $[0, c] \times [0, c]$. The constant c was chosen such that at very short times $P(\varphi_n, L, \Phi, \varepsilon, t)$ was close to one and no appreciable changes occurred in $P(\varphi_n, L, \Phi, \varepsilon, t)$ by increasing c further. We also checked that the curve for $(\varepsilon = 1/2, \Phi = \pi/2)$, for which we know the propagator exactly [see (43)], was accurately reproduced. In all the curves having reached the asymptotic regime, the long time values are in very good agreement with the ones given by the relations (74)–(76).

n dependence. One sees in Fig. 6 that $P(\varphi_n, L, \Phi, \varepsilon, t)$ decreases with n at all times and that at large times $P(\varphi_n, L, \Phi, \varepsilon, t) \sim C(\varphi_n, L, \Phi, \varepsilon)/t^3$ in good agreement with (74).

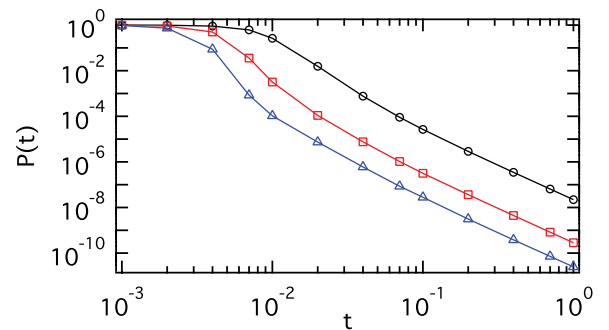


FIG. 6. (Color online) Log-log plot of $P(\varphi_n, L, \Phi, \varepsilon, t)$ as a function of time t for $L = 1$, $\varepsilon = 1/2$, $\Phi = \pi/2$, and $n = 1$ (black circle), $n = 2$ (red square), and $n = 3$ (blue triangle).

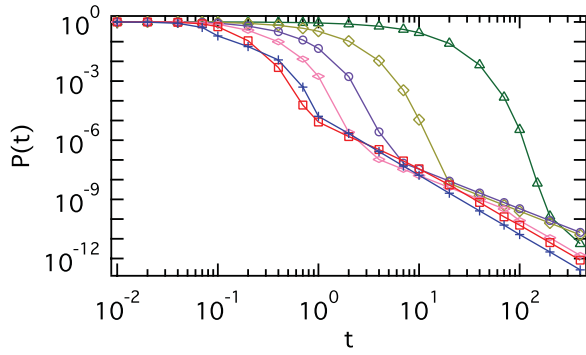


FIG. 7. (Color online) Log-log plot of $P(\varphi_n, L, \Phi, \varepsilon, t)$ as a function of time t for $n = 1$, $L = 1$, $\varepsilon = 1/2$, and $\Phi = 0.1$ (green triangle), $\Phi = 0.3$ (yellow diamond), $\Phi = 0.5$ (purple circle), $\Phi = 0.7$ (pink lozenge), $\Phi = 1$ (red square), and $\Phi = 2$ (blue cross).

Φ dependence. The Φ dependence of $P(\varphi_n, L, \Phi, \varepsilon, t)$ is represented in Figs. 7–9. In the curves having reached the asymptotic regime, one sees that $P(t) \sim C(\varphi_n, L, \Phi, \varepsilon)/t^3$ at large times, where the constant $C(\varphi_n, L, \Phi, \varepsilon)$ decreases with Φ when $\Phi \in (0, 2.33)$ (see Fig. 7) and increases when $\Phi \in (2.33, 2\pi)$ (see Fig. 8), as expected from Fig. 4. Note, however, that there may be several crossing among the curves. Note that similar features were obtained in a circular dielectric cavity containing classical waves [19]. In Fig. 9, one sees that $\Phi = 2\pi$ leads to $P(\varphi_n, L, \Phi, \varepsilon, t) \sim C(\varphi_n, L, \Phi, \varepsilon)/t$ as expected from (75), while $\Phi = \pi, 3\pi, 4\pi$ lead to $P(\varphi_n, L, \Phi, \varepsilon, t) \sim C(\varphi_n, L, \Phi, \varepsilon)/t^3$ as expected from (74) and (76).

ε dependence. In Fig. 10, one sees that $P(\varphi_n, L, \Phi, \varepsilon, t) \sim C(\varphi_n, L, \Phi, \varepsilon)/t^3$ at large times and that the constant $C(\varphi_n, L, \Phi, \varepsilon)$ increases with ε . On the other hand, note that $P(\varphi_n, L, \Phi, \varepsilon, t)$ decreases with ε at short times and that the curves cross each other.

Exponential decay. Plotting the curves in Figs. 6–10 on a log-lin plot (not shown) reveals that on some intermediate time scale (not very small and not very large), the nonescape probability decays approximately as an exponential, in agreement with [7].

VI. THE INTERACTING CASE

So far we have solely discussed the free evolution. To have an idea about the interacting evolution, let us consider the case

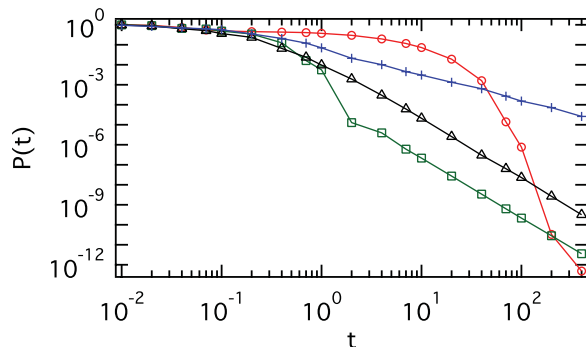


FIG. 8. (Color online) Log-log plot of $P(\varphi_n, L, \Phi, \varepsilon, t)$ as a function of time t for $n = 1$, $L = 1$, $\varepsilon = 1/2$, and $\Phi = 3$ (red circle), $\Phi = 4$ (green square), $\Phi = 5$ (black triangle), and $\Phi = 6$ (blue cross).

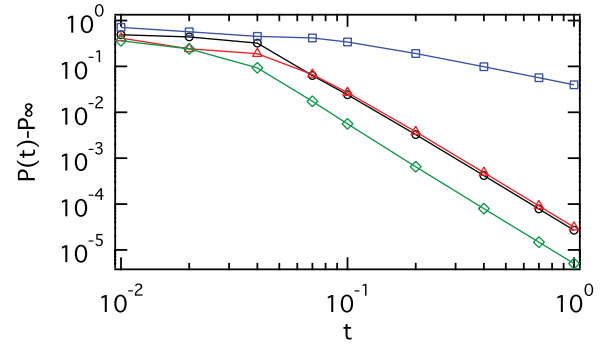


FIG. 9. (Color online) Log-log plot of $P(\varphi_n, L, \Phi, \varepsilon, t) - P_\infty(\varphi_n, \Phi)$ as a function of time t for $n = 1$, $L = 1$, $\varepsilon = 1/2$, and $\Phi = \pi$ (black circle), $\Phi = 2\pi$ (blue square), $\Phi = 3\pi$ (red triangle), and $\Phi = 4\pi$ (green diamond).

$\Phi = 0$ and $\varepsilon = 4/9$, where the Hamiltonian of the particle is given by

$$H = H_0 + V(Q). \quad (80)$$

Here $H_0 = -\frac{d^2}{dx^2}$ is the free Hamiltonian and V is the potential which for simplicity is supposed to be bounded, so that the Hamiltonian H is self-adjoint in the domain $D(H)$ specified by the conditions (16)–(18) with $\varepsilon = 4/9$.

Obviously, in this case the time-dependent Schrödinger equation (21) cannot be solved analytically in general and it also seems extremely difficult to compute analytically the large time behavior of the nonescape probability, so we shall consider a fully numerical approach. For this, let us consider a long but finite lead of length $\ell > L$ and set $\psi(L + \ell) = 0$. The assumption $\ell > L$ is natural in our case and also simplifies the remaining discussion. One can then check that H is self-adjoint in

$$D(H) = \{\psi \in \mathcal{H} \mid H\psi \in \mathcal{H} \text{ and (82)–(84) are satisfied}\}, \quad (81)$$

where

$$\psi(0_+) = \psi(L_-) = \psi(L_+), \quad (82)$$

$$\psi'(L_-) = \psi'(0_+) + \psi'(L_+), \quad (83)$$

$$\psi(L + \ell) = 0. \quad (84)$$

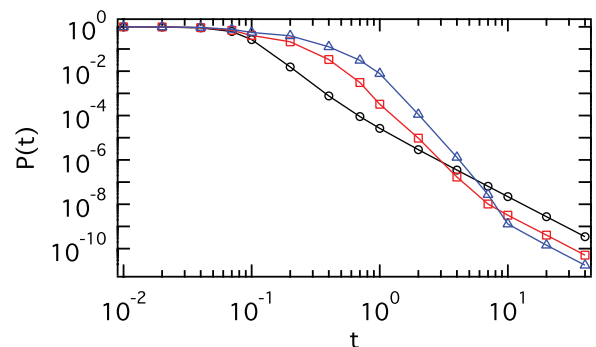


FIG. 10. (Color online) Log-log plot of $P(\varphi_n, L, \Phi, \varepsilon, t)$ as a function of time t for $n = 1$, $L = 1$, $\Phi = \pi/2$, and $\varepsilon = 0.3$ (blue triangle), $\varepsilon = 0.4$ (red square), and $\varepsilon = 0.5$ (black circle).

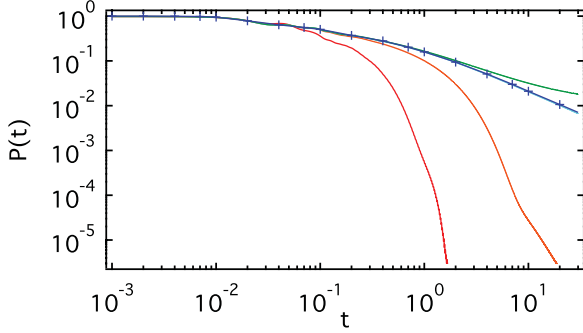


FIG. 11. (Color online) The nonescape probability $P(\psi_0, L, \ell, \lambda, t)$ as a function of time t for a soft-core Coulomb potential by using the pseudospectral method with $L = 1$, $\ell = 500$, $\Delta x = 1/80$, $\Delta t = 10^{-3}$. (From top to bottom) $\lambda = -0.1$ (green), $\lambda = 0$ (light blue), $\lambda = 0.1$ (orange), and $\lambda = 1$ (red). The dark blue cross curve (close to the $\lambda = 0$ curve) corresponds to the free case ($V = 0$) with $\ell = \infty$ and is obtained by using the expression (79).

Clearly, for our numerical results to remain accurate for a long time the unitarity of the time evolution is crucial. A convenient way to implement numerically the boundary conditions (82)–(84), while preserving unitarity, is to use the pseudospectral method presented in Appendix D. This method requires the knowledge of the spectrum and bound states of the free Hamiltonian H_0 , which are worked out in Appendix E. We believe that this section and the Appendices D and E present, in particular, an interesting and highly nontrivial application of the pseudospectral method.

Let us consider the following initial state:

$$\psi_0(x) = \sqrt{\frac{8}{3L}} \sin^2\left(\frac{2\pi}{L}x\right) \chi_{[0,L]}(x). \quad (85)$$

It is easy to check that ψ_0 is normalized ($\|\psi_0\| = 1$) and belongs to $D(H)$. Note that ψ_0 is an even function in $L^2([0, L])$ and thus it is orthogonal to all bound states of the loop. Therefore, in the infinite case $\ell = \infty$ with no potential ($V = 0$), the nonescape probability will vanish at large times and the asymptotic decay can be computed by using (66)

$$P_{\text{free}}(\psi_0, L, \ell = \infty, t) = \frac{2L^2}{3\pi} \frac{1}{t} + O\left(\frac{1}{t^2}\right). \quad (86)$$

Numerically, the infinite situation ($\ell = \infty$) is obtained by using the expression (79) and gives the dark blue cross curve in Fig. 11. Its asymptotic values are in very good agreement with formula (86). On the other hand, the finite case ($\ell < \infty$) is obtained by using the pseudospectral method and leads to the light blue curve in Fig. 11. As one clearly sees, the two methods are in very good agreement.

Imagine now that a fictive charged particle is fixed at the point $x = L/2$ (i.e., at the leftmost part of the loop) and interacts with our genuine charged particle via a soft-core Coulomb force. Then, a simple calculation leads to the

following potential ($0 \leq x \leq L + \ell$):

$$V_\lambda(x) = \frac{\lambda}{\sqrt{d(x)^2 + 10^{-4}}},$$

$$d(x) = \begin{cases} \sqrt{2R} \sqrt{1 - \cos\left(\pi - \frac{x}{R}\right)} & \text{if } x \leq L, \\ 2R + x - L & \text{if } x > L, \end{cases} \quad R = \frac{L}{2\pi}. \quad (87)$$

When $\lambda > 0$, the force is repulsive, while $\lambda < 0$ corresponds to an attractive force. The numerical results are presented in Fig. 11. As expected, we see that $P(\psi_0, L, \ell, \lambda, t)$ decays faster than the free case if $\lambda > 0$ and slower if $\lambda < 0$. Note also that globally the curves look similar to the ones obtained in the free cases presented in the previous section. In particular, plotting these curves on a log-lin plot (not shown) reveals the approximate exponential decay on some intermediate time scale. Although our numerical results do not show any asymptotic power law decay when $\lambda \neq 0$, such a regime may well be present at larger times. To reach larger times, however, one has to increase the length of the lead ℓ (because the particle gets reflected at the end of the lead and comes back into the loop causing a bump in the curves after some time) but this increases the computation time very quickly.

VII. CONCLUDING REMARKS

Although more energetic bound states typically escape faster from the loop, we found that different bound states may actually decay with different power laws and consequently it may be possible to filter one bound state from a coherent superposition by applying the appropriate magnetic flux Φ through the loop. Indeed, suppose that the system is prepared such that at time $t = 0$ no magnetic flux crosses the loop and the particle is in the state,

$$\psi_0 = \sum_{n=1}^{\infty} c_n \varphi_n, \quad (88)$$

satisfying $\|\psi_0\| = 1$, where φ_n are the bound states (72). Then, if one wants to *filter* the bound state φ_m , one may apply a magnetic flux $\Phi = 2m\pi$ through the loop for a sufficiently long time, so that the state φ_m decays as $1/t$ while all the others decay as $1/t^3$ [see (75)–(76)].

The short-time behavior of $P(\psi_0, L, \Phi, \varepsilon, t)$ is also interesting and can be conveniently written as $P(\psi_0, L, \Phi, \varepsilon, t) = 1 - \|\chi_{[L, \infty)}(Q)e^{-iHt}\psi_0\|^2$. By computing the propagator $K(x, y, t)$ for $x > L$ and $y < L$, one then finds that $P(\psi_0, L, \Phi, \varepsilon, t) = 1 - D_2(\psi_0, L, \Phi, \varepsilon)t^2 + O(t^3)$ as $t \rightarrow 0$. In general, it seems that the constant $D_2(\psi_0, L, \Phi, \varepsilon)$ cannot be expressed in a simple form and thus its behavior would require a refined numerical investigation.

To make more apparent the exponential decay of the nonescape probability at intermediate times, while keeping the power law decay explicit at large times, it would be interesting to write $P(\psi_0, L, \Phi, \varepsilon, t)$ as $P_\infty(\psi_0, \Phi) + A(\psi_0, L, \Phi, \varepsilon) \exp[-\alpha(\psi_0, L, \Phi, \varepsilon)t] + \sum_{k=1}^{\infty} B_k(\psi_0, L, \Phi, \varepsilon)/t^k$ and to determine the unknown variables A , α , and B_k . One may also analyze the transition times between the exponential regime and the power law

regime with respect to the parameters ε and Φ , and also λ if there is such a transition.

A very interesting and challenging problem is to obtain a thorough description of the long-time behavior of the nonescape probability in the interacting case. It is clear that one would have to proceed analytically and thus in general it would be highly nontrivial. Basically, the problem consists in finding out a nontrivial class of potentials V , such as short-range potentials, for which the asymptotic decay rate of the nonescape probability can be effectively deduced (see [6] and references therein).

ACKNOWLEDGMENTS

The author thanks T. Taniguchi for suggesting this problem and for stimulating discussions. He also thanks W. O. Amrein, M. Büttiker, J.-P. Eckmann, P. Exner, J. Jacquet, Ph. Jacquod, and C.-A. Pillet for helpful comments and E. Hairer and C. Lubich for useful remarks related to the numerical simulations. This work was partially supported by the Japan Society for the Promotion of Science.

APPENDIX A: PROPERTIES OF THE HAMILTONIAN H

Here we show that the Hamiltonian H is self-adjoint in $D(H)$ given in (19). First of all, it is clear that $D(H)$ is dense in \mathcal{H} , so that the adjoint H^* of H is well defined. Let us recall that an operator $\{H, D(H)\}$ is self-adjoint if $D(H^*) = D(H)$ and $H^*\psi = H\psi$ for all $\psi \in D(H)$, where a vector $f \in \mathcal{H}$ belongs to $D(H^*)$ if there is a vector $f^* \in \mathcal{H}$ such that $\langle f|Hg \rangle = \langle f^*|g \rangle$ for all $g \in D(H)$, and for each $f \in D(H^*)$ one sets $H^*f = f^*$.

Let $f \in \mathcal{H}$ be a vector such that $Hf \in \mathcal{H}$ and let $g \in D(H)$. Then,

$$\langle f|Hg \rangle = \langle Hf|g \rangle + \text{BT}, \tag{A1}$$

where

BT

$$\begin{aligned} &= 2i \frac{\Phi}{L} g(0_+) [\overline{f(L_-)} - \overline{f(0_+)}] - \frac{g(0_+)}{b} \{\sqrt{\varepsilon} f'(L_+)\} \\ &+ b [\overline{f'(0_+)} - \overline{f'(L_-)}] + \frac{g'(0_+)}{\sqrt{\varepsilon}} [\sqrt{\varepsilon} f(0_+) - b \overline{f(L_+)}] \\ &- \frac{g'(L_-)}{\sqrt{\varepsilon}} [\sqrt{\varepsilon} f(L_-) - b \overline{f(L_+)}]. \end{aligned}$$

Here we have used the fact that $g \in D(H)$. We see that BT vanishes for all $g \in D(H)$ if and only if f also satisfies the boundary conditions (16)–(18). This shows that $D(H^*) = D(H)$ and $H^*f = Hf$ for all $f \in D(H)$ (i.e., H is self-adjoint).

Let us now show that the spectrum $\sigma(H)$ of H is $[0, \infty)$. Since H is self-adjoint, it follows that $\sigma(H) \subset \mathbb{R}$. Writing $H = P_\Phi^2$, with $P_\Phi = -i \frac{d}{dx} - \frac{\Phi}{L} \chi_{[0,L]}(Q)$, one easily shows that $\langle \varphi|H\varphi \rangle = \|P_\Phi \varphi\|^2 \geq 0$ for all $\varphi \in D(H)$. This means that H is a positive operator and thus $\sigma(H) \subset [0, \infty)$. Let $k > 0$ be fixed, then a (particular) solution of $H\varphi = k^2\varphi$ is

$$\varphi(x) = e^{ik(x-L)} \chi_{[L, \infty)}(x). \tag{A2}$$

Take $\psi \in C_0^\infty(\mathbb{R})$ satisfying $\psi(0) = \psi'(0) = 0$ and $\int_0^\infty |\psi(y)|^2 dy = 1$, and set

$$\psi_n(x) = \frac{1}{\sqrt{n}} \psi\left(\frac{x-L}{n}\right) \varphi(x), \tag{A3}$$

where $x > 0$ and $n = 1, 2, \dots$

It is easy to check that $\psi_n \in D(H)$ and $\|\psi_n\| = 1$ for all n , and that $\|H\psi_n - k^2\psi_n\| \rightarrow 0$ as $n \rightarrow \infty$. This shows that $E = k^2 > 0$ belongs to the spectrum of H (see Prop. 4.20 in [27] or Th. 2.2.1 in [28]). Since $k > 0$ is arbitrary and the spectrum of H is a closed set, one can conclude that $\sigma(H) = [0, \infty)$.

APPENDIX B: THE COEFFICIENTS $A, B, C,$ AND D

The denominator $\Omega(k)$ of the coefficients (24)–(27) vanish if and only if

$$a^2 \sin^2(kL) + b^2 [\cos(kL) - \cos(\Phi)]^2 = 0. \tag{B1}$$

Since a and b are always nonzero (remember that $\varepsilon = 0$ is excluded) the above equality is satisfied if and only if

$$\sin(kL) = 0 \quad \text{and} \quad \cos(kL) = \cos(\Phi). \tag{B2}$$

The first relation is verified only if $kL = n\pi$, for some $n \in \mathbb{Z}$, and consequently the second relation reads $\cos(\Phi) = (-1)^n$. This shows that the coefficients $A, B, C,$ and D may contain singularities only if $\cos(\Phi) = 1$ or $\cos(\Phi) = -1$. We shall now discuss these two cases separately.

(1) Case $\cos(\Phi) = 1$ or $\Phi = 2n\pi$, with $n \in \mathbb{Z}$. Using trigonometric relations, one may write

$$\begin{aligned} A(k) = -\overline{B(k)} &= -\sqrt{\frac{\varepsilon}{8\pi}} \\ &\times \frac{\sqrt{1 - \cos(kL)} + i \operatorname{sgn}[\sin(kL)] \sqrt{1 + \cos(kL)}}{\{a^2[1 + \cos(kL)] + b^2[1 - \cos(kL)]\}^{1/2}}. \end{aligned} \tag{B3}$$

Since the denominator of this expression is always nonzero, it follows that A and B are well defined in \mathbb{R} . Next, one may write

$$C(k) = -\overline{D(k)} = -\frac{1}{2b\sqrt{\varepsilon}} [2(b - \varepsilon)A(k) - 2bB(k)], \tag{B4}$$

showing that C and D are also well defined in \mathbb{R} . Furthermore, one has

$$f_1(k) = \frac{\varepsilon}{4\pi \{a^2[1 + \cos(kL)] + b^2[1 - \cos(kL)]\}}, \tag{B5}$$

$$f_2(k) = \frac{e\varepsilon^{-ikL}}{4\pi \{a^2[1 + \cos(kL)] + b^2[1 - \cos(kL)]\}}. \tag{B6}$$

(2) Case $\cos(\Phi) = -1$ or $\Phi = (2n + 1)\pi$, with $n \in \mathbb{Z}$. In this case, the relation (B4) still holds with

$$\begin{aligned} A(k) = -\overline{B(k)} &= -\sqrt{\frac{\varepsilon}{8\pi}} \\ &\times \frac{\sqrt{1 + \cos(kL)} - i \operatorname{sgn}[\sin(kL)] \sqrt{1 - \cos(kL)}}{\{a^2[1 - \cos(kL)] + b^2[1 + \cos(kL)]\}^{1/2}}. \end{aligned} \tag{B7}$$

Therefore, the coefficients are also well defined in this case and we have

$$f_1(k) = \frac{\varepsilon}{4\pi \{a^2[1 - \cos(kL)] + b^2[1 + \cos(kL)]\}}, \quad (\text{B8})$$

$$f_2(k) = \frac{-\varepsilon e^{-ikL}}{4\pi \{a^2[1 - \cos(kL)] + b^2[1 + \cos(kL)]\}}. \quad (\text{B9})$$

APPENDIX C: THE IDENTITY (48)

Here we show the identity (48). From the equality,

$$\int_{-\infty}^{\infty} e^{-ak^2+bk} dk = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}, \quad (\text{C1})$$

one can write

$$\int_{-\infty}^{\infty} k^n e^{-ak^2+bk} dk = \sqrt{\frac{\pi}{a}} \frac{d^n}{db^n} \left(e^{\frac{b^2}{4a}} \right). \quad (\text{C2})$$

One then concludes by using the following formula for the Hermite polynomial:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2}) = \sum_{\ell=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!(-1)^\ell}{\ell!(n-2\ell)!} (2x)^{n-2\ell}. \quad (\text{C3})$$

APPENDIX D: THE PSEUDOSPECTRAL METHOD

In Appendix E, we show that the free Hamiltonian H_0 has a pure point spectrum $\{E_n\}_{n=1}^{\infty}$ satisfying $0 < E_1 < E_2 < \dots$ (so each eigenvalue is positive and has multiplicity 1), and that one can solve (explicitly) the free stationary Schrödinger equation,

$$H_0\varphi_n = E_n\varphi_n, \quad (\text{D1})$$

with $\varphi_n \in D(H_0) = D(H)$ and $\|\varphi_n\| = [\int_0^{L+\ell} |\varphi_n(x)|^2 dx]^{1/2} = 1$. Let $\psi_0 \in D(H)$, $x \in [0, L + \ell]$, and $\Delta t > 0$, then

$$\psi(x, \Delta t) = (e^{-iH\Delta t} \psi_0)(x). \quad (\text{D2})$$

Let us consider the symmetric decomposition known as Strang splitting ($H = H_0 + V$):

$$e^{-iH\Delta t} = e^{-iV\Delta t/2} e^{-iH_0\Delta t} e^{-iV\Delta t/2} + O(\Delta t^3). \quad (\text{D3})$$

Since $\{\varphi_n\}_{n \geq 1}$ forms an orthonormal basis of the Hilbert space \mathcal{H} , one can write

$$e^{-iV\Delta t/2} \psi_0 = \sum_{n=1}^{\infty} \langle \varphi_n | e^{-iV\Delta t/2} \psi_0 \rangle \varphi_n. \quad (\text{D4})$$

Substituting (D3) and (D4) in (D2) gives

$$\begin{aligned} \psi(x, \Delta t) &= \sum_{n=1}^{\infty} e^{-iE_n\Delta t} e^{-iV(x)\Delta t/2} \varphi_n(x) \\ &\quad \times \int_0^{L+\ell} e^{-iV(y)\Delta t/2} \overline{\varphi_n(y)} \psi_0(y) dy + O(\Delta t^3). \end{aligned} \quad (\text{D5})$$

Let $\Phi \in \mathcal{H}$, and let us define a generalized Fourier transform \mathcal{F} as ($n = 1, 2, \dots$),

$$\hat{\Phi}(n) = \mathcal{F}(\Phi)(n) = \int_0^{L+\ell} \overline{\varphi_n(y)} \Phi(y) dy. \quad (\text{D6})$$

Since the family $\{\varphi_n\}_{n \geq 1}$ forms an orthonormal basis of \mathcal{H} , we have the following:

$$\Phi(x) = \mathcal{F}^{-1}(\hat{\Phi})(x) = \sum_{m=1}^{\infty} \varphi_m(x) \hat{\Phi}(m). \quad (\text{D7})$$

One may then rewrite (D5) as

$$\begin{aligned} \psi(x, t + \Delta t) &= e^{-iV(x)\Delta t/2} \mathcal{F}^{-1} [e^{-iE_n\Delta t} \\ &\quad \times \mathcal{F}(e^{-iV(\cdot)\Delta t/2} \psi(\cdot, t))] (x) + O(\Delta t^3). \end{aligned} \quad (\text{D8})$$

This relation is a common way of presenting the pseudospectral method. Numerically, the Fourier transform and its inverse are then computed by using a very efficient algorithm known as the fast Fourier transform (FFT). As far as we know, there is however no FFT using the eigenvectors $\{\varphi_n\}_{n \geq 1}$ of our model, so we shall compute $\psi(x, t + \Delta t)$ directly.

Let $\Delta x = (L + \ell)/N$, with $N \in \mathbb{N}$, be a small length difference, $x_k = k \Delta x$ the position of the k th site, with $k = 0, \dots, N$, $t_m = m \Delta t$, with $m = 0, 1, \dots$, and $\psi(\cdot, 0) = \psi_0$. Then, we will use the following relation in the numerical computation:

$$\begin{aligned} \psi(x_k, t_{m+1}) &= \sum_{n=1}^{\infty} e^{-iE_n\Delta t} e^{-iV(x_k)\Delta t/2} \varphi_n(x_k) \\ &\quad \times \int_0^{L+\ell} e^{-iV(y)\Delta t/2} \overline{\varphi_n(y)} \psi(y, t_m) dy + O(\Delta t^3). \end{aligned} \quad (\text{D9})$$

In the simulations, we consider only the first 2500 terms in the infinite sum occurring in (D9), compute the integral by using the composite Simpson rule, and check that probability is conserved at all times.

APPENDIX E: THE FREE HAMILTONIAN H_0

The free Hamiltonian H_0 is self-adjoint and thus its spectrum $\sigma(H_0) \subset \mathbb{R}$. Writing $H_0 = P^2$, with $P = -i \frac{d}{dx}$, one finds that $\langle \varphi | H_0 \varphi \rangle = \|P\varphi\|^2 \geq 0$ for all $\varphi \in D(H)$ and thus $\sigma(H_0) \subset [0, \infty)$. The general solution of $H_0\varphi_n = E_n\varphi_n$, with $E_n = k_n^2$ and $k_n \geq 0$, is

$$\begin{aligned} \varphi_n(x) &= [A_n e^{ik_n x} + B_n e^{-ik_n x}] \chi_{[0, L)}(x) \\ &\quad + [C_n e^{ik_n x} + D_n e^{-ik_n x}] \chi_{[L, L+\ell]}(x), \end{aligned} \quad (\text{E1})$$

where χ_I is the characteristic function of the interval I : $\chi_I(x) = 1$ if $x \in I$ and $\chi_I(x) = 0$ otherwise. Solving (82)–(84), one gets two types of solutions: First, we have the bound states of the loop ($C_n = D_n = 0$ and $A_n = -B_n$),

$$\begin{aligned} \varphi_m^{\text{loop}}(x) &= \sqrt{\frac{2}{L}} \sin(k_m^{\text{loop}} x) \chi_{[0, L)}(x), \\ k_m^{\text{loop}} &= \frac{2\pi m}{L}, \quad m = 1, 2, \dots \end{aligned} \quad (\text{E2})$$

Second, assuming that $k_n \neq k_m^{\text{loop}}$ for all $m = 1, 2, \dots$, we have

$$B_n = -\frac{1 - e^{ik_n L}}{1 - e^{-ik_n L}} A_n, \quad (\text{E3})$$

$$C_n = \frac{3 - 4e^{-ik_n L} + e^{-2ik_n L}}{2(1 - e^{-ik_n L})} A_n, \quad (\text{E4})$$

$$D_n = -\frac{3 - 4e^{ik_n L} + e^{2ik_n L}}{2(1 - e^{-ik_n L})} A_n, \quad (\text{E5})$$

$$k_n \neq \frac{(2s+1)\pi}{2\ell}, \quad s = 0, 1, 2, \dots \quad (\text{E6})$$

$$2 \tan(k_n \ell) = \frac{\sin(k_n L)}{1 - \cos(k_n L)}. \quad (\text{E7})$$

Explicitly, we thus have

$$\begin{aligned} \varphi_n^{\text{global}}(x) &= \frac{iA_n}{1 - e^{-ik_n L}} \{2[\sin(k_n x) - \sin(k_n(x-L))] \chi_{(0,L)}(x) \\ &\quad + [3\sin(k_n x) - 4\sin(k_n(x-L)) \\ &\quad + \sin(k_n(x-2L))] \chi_{[L, L+\ell]}(x)\}, \end{aligned} \quad (\text{E8})$$

where the coefficient A_n is determined by normalization: $\int_0^{L+\ell} |\varphi_n(x)|^2 dx = 1$. After some algebra, we found

$$\begin{aligned} A_n &= \left\{ 2L + \ell[5 - 3\cos(k_n L)] \right. \\ &\quad + 2 \frac{\sin(k_n L)[1 - 2\sin^2(k_n \ell)]}{k_n} \\ &\quad \left. + \frac{\sin(k_n \ell)\cos(k_n \ell)[5\cos(k_n L) - 3]}{k_n} \right\}^{-1/2}. \end{aligned} \quad (\text{E9})$$

It remains to solve (E7). As far as we can see, this relation cannot be solved explicitly. Since we shall sum up over the energies $E_n = k_n^2$, we actually only need to find out the non-negative solutions of (E7). Let $I_0 = [0, \frac{\pi}{2\ell}]$ and $I = [-\frac{\pi}{2\ell}, \frac{\pi}{2\ell}]$, and let us look for solutions of the following form:

$$k_n = n\frac{\pi}{\ell} + \delta_n, \quad (\text{E10})$$

where $n = 0, 1, 2, \dots$, $\delta_0 \in I_0$, $\delta_n \in I$, and such that $k_n \neq 2\pi m/L$ and $k_n \neq (2m+1)\pi/(2\ell)$ for all $m = 0, 1, 2, \dots$. Then, the relation (E7) reads

$$2 \tan(n\pi + \delta_n \ell) = \frac{\sin(n\frac{\pi L}{\ell} + \delta_n L)}{1 - \cos(n\frac{\pi L}{\ell} + \delta_n L)}. \quad (\text{E11})$$

Since $\tan(n\pi + \delta_n \ell) = \tan(\delta_n \ell)$, one finds

$$\delta_n = \frac{1}{\ell} \arctan \left[\frac{\sin(n\frac{\pi L}{\ell} + \delta_n L)}{2[1 - \cos(n\frac{\pi L}{\ell} + \delta_n L)]} \right], \quad (\text{E12})$$

where we consider the principal value of the arc-tangent function: $\arctan(\vartheta) \in (-\frac{\pi}{2}, \frac{\pi}{2})$. Note that $\cos(n\frac{\pi L}{\ell} + \delta_n L) \neq 1$, since $k_n \neq 2\pi m/L$ for all $m = 0, 1, 2, \dots$, so the above expression is well defined. Nevertheless, it will be convenient to attribute values to this expression on these exceptional points.

The condition $\cos(n\frac{\pi L}{\ell} + \delta_n L) = 1$ reads $n\frac{\pi L}{\ell} + \delta_n L = m2\pi$, with $m = 0, 1, 2, \dots$, or $\delta_n = m2\pi/L - n\pi/\ell$. Note that $\delta_0 \in I_0$ if and only if $m = 0$, since $\ell > L$, and thus $\delta_0 = 0$. For δ_n to belong to I , with $n \geq 1$, it is necessary that $|4m\ell/L - 2n| \leq 1$. Let us assume that ℓ/L is an integer (as in the simulation), then only the condition $|4m\ell/L - 2n| = 0$ or $\delta_n = 0$ might be satisfied, and thus any exceptional point δ_n must be at the center of I . Let us introduce the set $\Sigma = \{2m\ell/L \mid m = 1, 2, \dots\}$, which is the collection of n for which the condition $|4m\ell/L - 2n| = 0$, with $m = 1, 2, \dots$, is

satisfied. If $n \in \Sigma$, then we shall cut the interval I into two parts: $I = I^L \cup I^R$, where $I^L = [-\frac{\pi}{2\ell}, 0]$ and $I^R = [0, \frac{\pi}{2\ell}]$.

Let us define $F_0 : I_0 \rightarrow I_0$ as

$$F_0(\delta) = \frac{1}{\ell} \arctan \left[\frac{\sin(\delta L)}{2[1 - \cos(\delta L)]} \right], \quad (\text{E13})$$

and set $F_0(0) = \pi/(2\ell)$. If $n \geq 1$ and $n \notin \Sigma$, then we define $F_n : I \rightarrow I$ by

$$F_n(\delta) = \frac{1}{\ell} \arctan \left[\frac{\sin(n\frac{\pi L}{\ell} + \delta L)}{2[1 - \cos(n\frac{\pi L}{\ell} + \delta L)]} \right]. \quad (\text{E14})$$

On the other hand, if $n \in \Sigma$, we shall consider the functions $F^L : I^L \rightarrow I^L$ and $F^R : I^R \rightarrow I^R$ given by

$$F^L(\delta) = \frac{1}{\ell} \arctan \left[\frac{\sin(\delta L)}{2[1 - \cos(\delta L)]} \right], \quad (\text{E15})$$

$$F^R(\delta) = \frac{1}{\ell} \arctan \left[\frac{\sin(\delta L)}{2[1 - \cos(\delta L)]} \right], \quad (\text{E16})$$

and set $F^L(0) = -\pi/(2\ell)$ and $F^R(0) = \pi/(2\ell)$.

We shall show that F_0 , F_n , F^L , and F^R are contracting maps and thus, by the fixed point theorem, there exist unique points δ_0^* , δ_n^* , δ^{L*} , and δ^{R*} such that $F_0(\delta_0^*) = \delta_0^*$, $F_n(\delta_n^*) = \delta_n^*$, $F^L(\delta^{L*}) = \delta^{L*}$, and $F^R(\delta^{R*}) = \delta^{R*}$. Furthermore, these fixed points may be reached by iterations [e.g., $F_n^m(0)$, the m th iterate of F_n at point 0, converges to δ_n^* as $m \rightarrow \infty$]. This shows in particular that we have found all the solutions of (E12) and consequently of (E7), that H_0 has pure point spectrum and that each eigenvalue has multiplicity 1. Let us now show that F_n contracts; the proofs for F_0 , F^L , and F^R are similar. So let $X, Y \in I$ with $X \neq Y$. Then,

$$|F_n(X) - F_n(Y)| \leq C |X - Y|, \quad (\text{E17})$$

where

$$\begin{aligned} C &= \frac{|F_n(X) - F_n(Y)|}{|X - Y|} \leq \sup_{X \neq Y \in I} \frac{|F_n(X) - F_n(Y)|}{|X - Y|} \\ &\leq \sup_{X \in I} \left| \frac{dF_n}{dX}(X) \right| \leq \frac{L}{\ell} < 1. \end{aligned} \quad (\text{E18})$$

The last two inequalities follow from the assumption $L < \ell$ and the explicit computation of $F_n'(X)$:

$$\left| \frac{dF_n}{dX}(X) \right| = \frac{2L}{\ell[5 - 3\cos(n\frac{\pi L}{\ell} + LX)]}. \quad (\text{E19})$$

It remains to check that the fixed point δ_n^* of F_n gives rise to an allowed value of k_n , that is, satisfying $k_n \notin \{2\pi m/L, (2m+1)\pi/(2\ell)\}_{m=0}^{\infty}$. These conditions state that δ_n^* should not be a boundary value of I [i.e., $|\delta_n^*| \neq \pi/(2\ell)$]. This can be easily checked.

In the simulations, we iterate the map F_0 , F_n , F^L , and F^R until the condition (84) with $\psi = \varphi_n^{\text{global}}$ given in (E8) is accurately satisfied: We required that $|\varphi_n^{\text{global}}(L + \ell)| < 10^{-10}$. Since the contracting constant C is very small ($< L/\ell$), this condition is satisfied after only a few iterations. In summary, we have

$$k_0 = \delta_0^*, \quad \text{with } \delta_0^* \approx F_0 \circ \dots \circ F_0(\varepsilon), \quad (\text{E20})$$

$$n \notin \Sigma : k_n = n\frac{\pi}{\ell} + \delta_n^*, \quad \text{with } \delta_n^* \approx F_n \circ \dots \circ F_n(0), \quad (\text{E21})$$

$$n \in \Sigma : k_n^L = n \frac{\pi}{\ell} + \delta^{L*}, \quad \text{with } \delta^{L*} \approx F^L \circ \dots \circ F^L(-\varepsilon), \quad (\text{E22})$$

$$n \in \Sigma : k_n^R = n \frac{\pi}{\ell} + \delta^{R*}, \quad \text{with } \delta^{R*} \approx F^R \circ \dots \circ F^R(\varepsilon), \quad (\text{E23})$$

where ε is a small positive number [$\varepsilon < \pi/(2\ell)$]. The states can then be written as

$$\begin{aligned} \text{if } n \notin \Sigma : \quad & \varphi_n = \varphi_n^{\text{global}}, \\ \text{if } n \in \Sigma : \quad & \begin{cases} \varphi_n^L = \varphi_n^{\text{global}}, & \text{with } k_n = k_n^L \\ \varphi_n^C = \varphi_n^{\text{loop}}, & \text{with } k_n = \frac{n\pi}{\ell} \\ \varphi_n^R = \varphi_n^{\text{global}}, & \text{with } k_n = k_n^R. \end{cases} \quad (\text{E24}) \end{aligned}$$

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