Resonance tunneling of a classical particle

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Exact solutions are obtained for the diffusion in single- and square-well potentials, by using the Laplace transform method. We compare transmission of a classical particle through one barrier of given length and through two barriers with a well between them of the same overall length. It turns out that the existence of a well facilitates the transmission of a classical particle for intermediate times, which bears some resemblance to resonances tunneling through quantum barriers.

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The tunneling of a quantum particle through a potential barrier(s) is a well-known problem [1]. One of the peculiarities of this problem is a comparison of the transition through a double barrier [Fig. 1(b)] and a single barrier [Fig. 1(a)]. It turns out that the transmission coefficient for the incident particle can reach nearly unity for a double barrier, even though each of the barriers has a low transparency. This resonance phenomenon takes place when the energy of an incident particle is close to one of the eigenstates of a potential well that divides the two barriers.

A classical particle with energy smaller than the barrier's height is able to cross the barrier only in the presence of fluctuations. The question arises whether the existence of a potential well is able, as in the quantum case, to assist the transmission over the barrier. In contrast to the quantum case we consider a dynamic problem, comparing the time dependence of transmission of a classical particle through one barrier of given length and through two barriers with a well between them of the same overall length.

The potentials shown in Fig. 1 belong to the class of simple potentials when the exact solution of the full dynamic problem can be obtained by using the Laplace-transform of the Fokker-Planck equation for the probability distribution function P(x,t) of the form

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x} \left[\frac{1}{T} \frac{dU}{dx} P + \frac{\partial P}{\partial x} \right] \equiv -\frac{\partial J}{\partial x}, \tag{1}$$

where the diffusion coefficient D and the Bolzmann constant k are set equal to unity.

For the potentials shown in Fig. 1 $\frac{dU}{dx} = 0$ and Eq. (1) reduces to simple diffusion equation that can be easily solved in each of the intervals (-L, -a), (-a, -b), (-b, b), (b, a), and (a, L). The matching at the boundaries can be performed keeping in mind that the probability current J is continuous, while P(x,t) has finite jumps [2], $P(x-0,t)\exp(\frac{U(x-0)}{T}) = P(x+0,t)\exp(\frac{U(x+0)}{T})$ at the boundaries $x=\pm a$ and $x=\pm b$. We assume reflecting boundary conditions at the walls, $J(x=\pm L,t)=0$, or the vanishing of P(x,t) at $x=\pm \infty$ when the walls are absent [Figs. 1(c,d)].

For simplicity we assume that initially a particle is located at the very left end of the barrier,

$$P(x,t=0) = \delta(x+a) \tag{2}$$

although it is physically obvious that all qualitative results will not depend on the precise initial position of a particle in the interval (-L,-a). We have now completely defined the problem which can be solved using the Laplace transform, $P(x,s) = \int_0^\infty P(x,t) \exp(-st) dt$. In each of the intervals the solution has the form $C_i \exp(\sqrt{sx}) + C_{i+1} \exp(-\sqrt{sx})$, and one has to solve six matching equations for C_i , $i = 1, 2, \ldots 6$, for the potential shown in Figs. 1(a,c), and ten matching equations for those in Figs. 1(b,d).

We will report all details of these simple but tedious

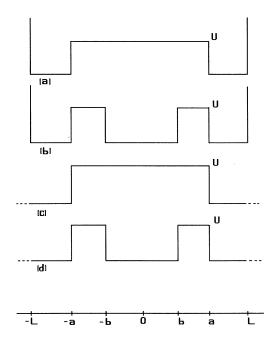


FIG. 1. Different forms of square-well potentials: (a) one barrier of width 2a and height U with reflecting boundaries at $x=\pm L$; (b) two barriers of width a-b and height U with a well of width 2b between the barriers and reflecting boundaries at $x=\pm L$; (c) the same as (a) with no boundaries; (d) the same as (b) with no boundaries.

calculations elsewhere, while here we use the important result for our purpose that the Laplace transform of the probability W(t) of finding a particle in the extreme right interval (a, L) in Fig. 1(b) after crossing the barriers is

$$\stackrel{\wedge}{W}(s) = \int_{a}^{L} \stackrel{\wedge}{P}(x,s) dx = rac{e^{rac{U}{T}} \sinh \left[2\sqrt{s}\left(L-a
ight)
ight]}{4s \mathcal{J}_{\mathrm{I}} \mathcal{J}_{\mathrm{II}}} \quad (3)$$

where the expressions \mathcal{J}_{I} and \mathcal{J}_{II} have the following form:

$$\begin{cases}
\mathcal{J}_{\text{I}} \\
\mathcal{J}_{\text{II}}
\end{cases} = \left\{ \cosh\left[r\left(L-a\right)\right] \sinh\left[r\left(a-b\right)\right] + e^{U/T} \sinh\left[r\left(L-a\right)\right] \cosh\left[r\left(a-b\right)\right] \right\} \times \left\{ \begin{array}{l} \cosh\left(rb\right) \\ \sinh\left(rb\right) \end{array} \right\} \\
+ e^{U/T} \left\{ \cosh\left[r\left(L-a\right)\right] \cosh\left[r\left(a-b\right)\right] + e^{U/T} \sinh\left[r\left(L-a\right)\right] \sinh\left[r\left(a-b\right)\right] \right\} \times \left\{ \begin{array}{l} \sinh\left(rb\right) \\ \cosh\left(rb\right) \end{array} \right\}, \tag{4}$$

where $r = \sqrt{s}$.

For $b \to 0$, the potential in Fig 1(b) reduces to that of Fig. 1(a), and, accordingly, Eqs. (3) and (4) describe the latter case when one puts b=0. For $L\to\infty$, Eqs. (3) and (4) describe the probability to be in the region (a,∞) after crossing the potential, Figs. 1(c,d).

Two types of poles exist in the inverse Laplace transform of Eq. (3): s=0, which defines the asymptotic behavior as $t\to\infty$, and those that come from the vanishing of $\mathcal{J}_{\rm I}$ and $\mathcal{J}_{\rm II}$. The inverse Laplace transform of (3), which contains in addition a branch point at s=0, is in itself nontrivial, and can be performed analytically only in a few cases where the characteristic lengths are the ratios of simple numbers.

We performed the inverse Laplace transform analytically for the following six cases for the potentials in Figs. 1(a) and 1(b): (1) L=2a, $b=\frac{a}{2}$; (2) $L=\frac{3a}{2}$, $b=\frac{a}{2}$; (3) $L=\frac{4a}{3}$, $b=\frac{a}{3}$, and for these values of L with b=0. In all these cases we calculated W(t) and found that the existence of a well inhibits the transmission, i.e., it is easier to pass one barrier than two. However, a more detailed analysis shows that the last statement is not always correct.

To clarify this point let us consider the asymptotic

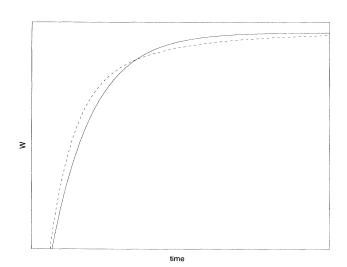


FIG. 2. Time dependence of the probability to find a particle in the interval (a,∞) after crossing one barrier [Fig. 1(c)] (solid line) and two barriers [Fig. 1(d)] (dashed line).

form of W(t) as $t \to \infty$, which can be obtained from the inverse Laplace transform of Eq. (3) for small s. The results turn out to be quite different for the unbounded motion in the potential in Fig. 1(d) and the restricted motion in the potential in Fig. 1(b). In the latter case,

1(b):
$$W(t)|_{t\to\infty} \sim \frac{e^{\frac{U}{T}} (L-a)}{2 \left[e^{\frac{U}{T}} (L-a) + e^{\frac{U}{T}} b + (a-b) \right]} + O\left(t^{-3/2}\right)$$
 (5)

while in the former one,

1(d):
$$W(t)|_{t\to\infty} \sim \frac{1}{2} - \frac{1}{\sqrt{\pi t}} \left[(a-b)\cosh(U_o/T) + b \right].$$
 (6)

An important difference between Eqs. (5) and (6) is that when $b \to 0$ the expression (6) decreases while (5) increases, i.e., it is easier for large t to pass two barriers than one for the unbounded motion in Figs. 1(c,d), and vice versa for Figs. 1(a,b). The explanation for the latter phenomenon is clear. Indeed, the stationary probability

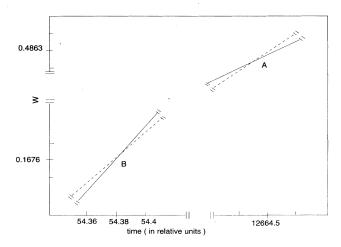


FIG. 3. Time dependence of the probability to find a particle in the interval (a,L) after crossing one barrier [Fig. 1(a); $L=100,\,a=3,\,b=0$] (solid line) and two barriers [Fig. 1(b); $L=100,\,a=3,\,b=0.1$] (dashed line).

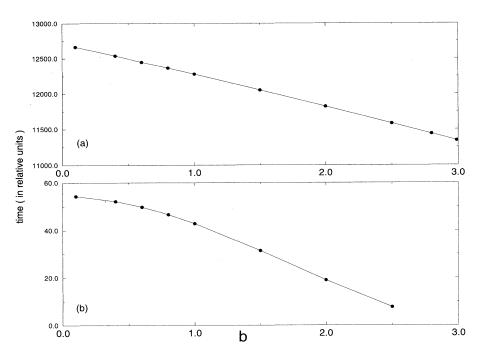


FIG. 4. Characteristic times in (relative units) that define the intersections of two curves for one and two barriers, with L=100 and a=3 as a function of the half-width of the well: (a) the large-time intersections (points A in Fig. 3); (b) the small-time intersections (points B in Fig. 3).

to be in the region (-b,b) is higher in the two-barrier case (as there is no barrier in this region), and, hence, the probability to be in the region of interest (a,L) is smaller compared with the one-barrier potential.

An analysis of another asymptotic case of small t [large s in (3)] when the reflection from the walls in Figs. 1(a,b) becomes important, shows that it is always (with an exception of the exponentially small barrier's width) easier to pass one barrier than two successive barriers.

Hence, for the unbounded motion [Figs. 1(c,d)] W(t) has the form shown in Fig. 2 with one intersection point between one- and two-barrier potentials.

The situation is more interesting for the restricted motion [Figs. 1(a,b)]. In both limit cases $t\to 0$ and $t\to \infty$, it is easier to pass one barrier than two. However, one can expect that for walls removed far away (which is quite similar to the unbounded case) there are some intermediate time intervals where it is easer to pass two barriers than one. Such points A and B shown in Fig. 3 were, indeed, founded in the numerical inverse Laplace transform. Figures 4(a,b) obtained for L=100, $\exp(\frac{U}{T})=5$, a=3 show two intersection points A and B as functions of the half-distance b between two barriers. We have not seen this effect in our exact solutions, since the distances to the reflecting walls were too small.

Jumps over high potential barriers are often described in the framework of the Kramers rate theory [3], which can be checked as soon as one knows the exact solution [2]. Following the well-known procedure [3] one finds the following expression for the Kramers rate k_r for the potential in Fig 1(b):

$$k_r = \frac{e^{-\frac{U}{T}}}{(L-a)(a-b)}.$$
 (7)

Notice that the Kramers rate is maximal when the width of a barrier, a-b, is equal to the distance L-a from the barrier to the reflecting wall. A comparison of Eq. (7) with asymptotic expansion in $\exp(-\frac{U}{T})$ of the inverse Laplace transform of Eq. (3) shows that for all exact solutions obtained, the smallest eigenvalues, indeed, coincide with k_r^{-1} , which justifies the applicability of the Kramers theory for the potentials shown in Fig. 1. As expected, the Kramers theory does not work for very narrow barriers.

In summary, we found that diffusion in simple potentials, like those shown in Fig. 1, contains some unexpected features, such as "resonant transmission" through double potential with a well in the middle, compared with a single potential of the same overall length.

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