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Time dependence and line shape of spontaneous quantum tunneling

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Abstract

The time dependence of spontaneous quantum tunneling of a particle from a potential well through a barrier in one or three dimensions is studied on the basis of the solution of the time-dependent Schrödinger equation as an initial-value problem by the method of Laplace transform. The wavefunction in the outer space is expressed in terms of special functions known from the theory of classical diffusion. A concise expression is derived for the probability current into the outer space. At long times the current oscillates about zero before decaying with a t^{-4} long-time tail. A comparison is made with the solution obtained by an expansion of the initial wavefunction in terms of the complete set of scattering states and bound states.

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1. Introduction

In quantum mechanics a particle, located initially in a region separated by a potential barrier from the rest of space, can escape the region, even if its energy is much less than the height of the barrier. The phenomenon was demonstrated by Hund [1] for internal rearrangements of molecules, such as ammonia. In early work on α -decay, Gamow [2] suggested that the rate of decay due to quantum tunneling could be calculated from the complex energy corresponding to an approximate solution of the time-independent Schrödinger equation. He used the WKB-method to find the approximate solution, and hence derived an expression for the rate [3]. It was argued by Born [4] and Casimir [5] that the dynamics of escape should be understood from the solution of the time-dependent Schrödinger equation, regarded as an initial-value problem. A thorough review of the theory developed in later years has been presented by Razavy [6].

In many situations in solid-state physics and chemistry the tunneling is stimulated by coupling to other degrees of freedom, such as phonons or molecular vibrations, causing dissipation and random forces. In such situations it is usually necessary to consider a thermal

ensemble of initial states. The corresponding theory has been reviewed by Hänggi *et al* [7], Weiss [8] and Nitzan [9].

Here we consider only the relatively simple case of spontaneous tunneling of a single particle under the influence of a fixed potential. The initial wavefunction is taken to be the ground state or an excited state for a modified potential, consisting of the original potential plus an infinite barrier confining the particle. The initial-value problem suggested by Born and Casimir was solved some years ago for simple model potentials by García-Calderón *et al* [10] and van Dijk and Nogami [11]. García-Calderón *et al* [10] expanded the wavefunction in the potential region for positive time in terms of Gamow states. van Dijk and Nogami [11] expanded the wavefunction in terms of the complete set of scattering solutions and bound states of the Hamilton operator. It is clear that in principle such an expansion provides the exact solution of the problem for all time. However, technical problems remain in the extraction of the desired information, such as the mean escape time.

In the following, we obtain the exact solution in a simplified form. The solution of van Dijk and Nogami [11] involves incoming waves, which seems counterintuitive in the description of the decay of a metastable state. We solve the initial-value problem by the method of Laplace transform. First, this has the advantage of a concise form for the solution. Second, it makes clear that the decay involves only outgoing waves and bound states. The connection with the solution of van Dijk and Nogami is made clear in section 6. In their solution the incoming waves serve to build up the initial state.

We also simplify the extraction of desired information on the time dependence of the probability of occupation of the well by concentrating on the probability current at the boundary with the outer space. The wavefunction in the outer space is expressed in terms of a sum of special functions which also appear in the related classical diffusion problem [12, 13], as described by the Smoluchowski equation. The special functions are related to the Moshinsky function [14].

The analysis is performed for the one-dimensional Schrödinger equation. By a well-known transformation it applies also in three dimensions for a centrally symmetric potential, provided the initial wavefunction is isotropic, i.e. for S -wave symmetry.

In general, the time dependence of the decaying occupation probability or occupancy is non-exponential. Although this is not surprising at short times, it is also true at long times, in contrast to the expectation of some [15]. At very long times the occupancy decays with a t^{-3} power law [16–18]. It was found by Winter [29] and van Dijk and Nogami [11] for specific models that the occupancy oscillates in time before the power law sets in. We confirm their finding and explain it as an interference phenomenon of sums of at least two fundamental wave modes.

Another approach to the tunneling problem has been proposed by Gurvitz [30], and further elaborated by Gurvitz *et al* [19]. The method is based on a different modified potential, and a different initial wavefunction than used here. The formalism presented here appears to be more straightforward. We show in sections 4 and 5 that for model potentials the resonance energy and half-width in the Breit–Wigner formula can be calculated exactly. The method of Gurvitz *et al* makes use of perturbation theory and yields an approximation to the exact result. The approach of Gurvitz *et al* has been extended to the many-body problem by Al-Khalili *et al* [20].

2. Escape from a one-dimensional potential

We consider the motion of a particle in one dimension in a potential $V(x)$, as described by the Schrödinger equation for the wavefunction $\psi(x, t)$. Putting $\hbar = 1$ we have for a particle of

mass m

$$i \frac{\partial \psi}{\partial t} = -\frac{1}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x, t). \quad (2.1)$$

We assume that the potential tends to $+\infty$ as $x \rightarrow -\infty$ and vanishes beyond a cutoff-point $c > 0$. We shall solve equation (2.1) as an initial-value problem for $t > 0$ for a given initial wavefunction $\psi(x, 0)$, constructed from an eigenfunction of a modified Hamiltonian operator $H_m = p^2/(2m) + V_m(x)$, with a modified potential $V_m(x)$. The modified potential $V_m(x)$ is identical with $V(x)$ for $x < c$, but leads to confinement and to a discrete set of eigenfunctions $\{\varphi_{mj}(x)\}$ with eigenvalues $\{E_{mj}\}$, enumerated by an index $j = 0, 1, 2, \dots$ according to ascending energy, starting with the ground state $\varphi_{m0}(x)$ at energy E_{m0} . For example, we require the potential $V_m(x)$ to tend to $+\infty$ at $x = c$, or we choose it to increase to $+\infty$ as a parabola for $x > c$. Thus, the function $\varphi_{mj}(x)$ satisfies the time-independent Schrödinger equation

$$-\frac{1}{2m} \frac{d^2 \varphi_{mj}}{dx^2} + V_m(x)\varphi_{mj}(x) = E_{mj}\varphi_{mj}(x) \quad (2.2)$$

on the interval $-\infty < x < c$, or even on the interval $-\infty < x < \infty$. The initial wavefunction is chosen as

$$\begin{aligned} \psi(x, 0) &= \varphi_{mj}(x) & \text{for } x < c, \\ &= 0 & \text{for } x > c. \end{aligned} \quad (2.3)$$

The function is taken to be real. In most of our examples, we shall consider the ground state $\varphi_{m0}(x)$.

We solve the Schrödinger equation (2.1) by Laplace transform. It is convenient to consider the complex conjugate wavefunction $\psi^*(x, t)$. We write

$$f(x, t) = \psi^*(x, t) \quad (2.4)$$

in order to avoid confusion with the asterisk. The Laplace transform is defined as

$$\hat{f}(x, s) = \int_0^\infty e^{-st} f(x, t) dt. \quad (2.5)$$

Then, $\hat{f}(x, s)$ satisfies the equation

$$is \hat{f}(x, s) = v \frac{d^2 \hat{f}(x, s)}{dx^2} - V(x)\hat{f}(x, s) + i\psi(x, 0), \quad (2.6)$$

with $v = 1/(2m)$. Since both $V(x)$ and $\psi(x, 0)$ vanish for $x > c$, the solution for this region can be written as

$$\hat{f}(x, s) = B e^{-ik(x-c)}, \quad \text{for } x > c \quad (2.7)$$

with $k = -i\sqrt{is/v}$ and s -dependent coefficient B . The variable k is defined such that $B(s)$ has a branch cut along the positive imaginary axis in the complex s plane. With $\psi(x, 0)$ given by equation (2.3), a solution of the inhomogeneous differential equation (2.6) for $x < c$ is given by

$$\phi(x, s) = \frac{1}{s - iE_{mj}} \varphi_{mj}(x). \quad (2.8)$$

Therefore, the solution of equation (2.6) satisfying the boundary condition at $x = -\infty$ takes the form

$$\hat{f}(x, s) = \phi(x, s) + A f_r(x, s), \quad \text{for } x < c, \quad (2.9)$$

where $f_r(x, s)$ is a solution of the homogeneous differential equation which tends to zero as $x \rightarrow -\infty$. The normalization of the latter solution may be chosen conveniently. The coefficients A in equation (2.9) and B in equation (2.7) are determined from the conditions that $\hat{f}(x, s)$ and its derivative with respect to x are continuous at $x = c$. This yields

$$A = \frac{1}{s - iE_{mj}} \frac{-ik\varphi_{mj}(c) - \varphi'_{mj}(c)}{f'_r(c, s) + ikf_r(c, s)}, \tag{2.10}$$

$$B = \frac{1}{s - iE_{mj}} \frac{f'_r(c, s)\varphi_{mj}(c) - f_r(c, s)\varphi'_{mj}(c)}{f'_r(c, s) + ikf_r(c, s)},$$

where the prime denotes the derivative with respect to x . Clearly, the coefficient B is independent of the normalization chosen for the function $f_r(x, s)$. The wavefunction $f(x, t)$ is given by the inverse Laplace transform

$$f(x, t) = \frac{1}{2\pi i} \int_{-i\infty+\varepsilon}^{i\infty+\varepsilon} e^{st} \hat{f}(x, s) ds, \tag{2.11}$$

with ε sufficiently positive so that the path of integration in the complex s plane is to the right of all singularities of the integrand.

In particular, for $x > c$

$$f(x, t) = \frac{1}{2\pi i} \int_{-i\infty+\varepsilon}^{i\infty+\varepsilon} B(s) e^{-ik(x-c)+st} ds \quad (x > c). \tag{2.12}$$

With the change of variables $s = -i\omega$ the inverse Laplace transform in equation (2.11) may also be expressed as the Fourier transform

$$f(x, t) = \frac{1}{2\pi} \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} e^{-i\omega t} \hat{f}(x, -i\omega) d\omega. \tag{2.13}$$

In the outer region $x > c$

$$f(x, t) = \frac{1}{2\pi} \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} B(-i\omega) e^{-ik(x-c)-i\omega t} d\omega \quad (x > c) \tag{2.14}$$

where $k = -i\sqrt{\omega/v}$. The integrand has a branch cut along the negative real ω axis.

From the conjugate wavefunction $f(x, t)$ in the outer region, we can evaluate the occupancy $P(t)$ of the inner region from

$$P(t) = 1 - \int_c^\infty |f(x, t)|^2 dx, \tag{2.15}$$

since probability is conserved. In earlier works [6, 10, 11] the quantity $P(t)$ has been called the nonescape probability, but we avoid this nomenclature, since before time t the particle can escape and return to the inner region any number of times. The occupancy $P(t)$ equals unity at $t = 0$. In case there are bound states it tends to a constant P_∞ , otherwise it tends to zero as $t \rightarrow \infty$. The mean escape time τ_M may be defined by

$$\tau_M = \int_0^\infty (P(t) - P_\infty) dt / (1 - P_\infty). \tag{2.16}$$

In general, the decay is non-exponential.

In order to calculate the survival probability

$$S(t) = \left| \int_{-\infty}^c \psi(x, t) \psi(x, 0) dx \right|^2 \tag{2.17}$$

one needs the wavefunction in the inner region. In examples this can be evaluated as well by the use of equation (2.9). We recall that we have chosen the initial wavefunction $\psi(x, 0)$ to be real.

In order to calculate the time-dependent occupancy $P(t)$, it is not necessary to perform the integration in equation (2.15). As a consequence of the Schrödinger equation the rate of change is given by

$$\frac{dP}{dt} = -J(t), \tag{2.18}$$

with probability current at $x = c$

$$J(t) = \frac{1}{2mi} \left[\psi^*(x, t) \frac{\partial \psi(x, t)}{\partial x} - \psi(x, t) \frac{\partial \psi^*(x, t)}{\partial x} \right] \Big|_{x=c}. \tag{2.19}$$

Thus, it is sufficient to evaluate the wavefunction and its spatial derivative at the exit point $x = c$. We abbreviate

$$F(t) = f(c, t), \quad G(t) = -\frac{\partial}{\partial x} f(x, t) \Big|_{x=c}. \tag{2.20}$$

With this notation

$$J(t) = 2v \Im F^*(t)G(t). \tag{2.21}$$

By the use of Parseval's theorem [21]

$$1 - P_\infty = \frac{v}{\pi} \Im \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \hat{F}^*(-i\omega) \hat{G}(-i\omega) d\omega. \tag{2.22}$$

Here and in the following the limit $\varepsilon \rightarrow 0+$ is understood. The functions $\hat{F}(-i\omega)$ and $\hat{G}(-i\omega)$ are related by

$$\hat{F}(-i\omega) = B(-i\omega), \quad \hat{G}(-i\omega) = \sqrt{\omega/v} B(-i\omega), \tag{2.23}$$

so that we can rewrite equation (2.22) as

$$1 - P_\infty = \frac{\sqrt{v}}{\pi} \Im \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \sqrt{\omega} |B(-i\omega)|^2 d\omega. \tag{2.24}$$

The square root has an imaginary part on the negative frequency axis, so that we can rewrite this as

$$1 - P_\infty = \int_0^\infty g(E) dE, \tag{2.25}$$

where

$$g(E) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\pi} \sqrt{vE} |B(iE + \varepsilon)|^2 \tag{2.26}$$

may be interpreted as the energy spectrum of the decay.

Alternatively, the mean escape time may be defined from

$$(1 - P_\infty) \tau_M = \int_0^\infty t J(t) dt. \tag{2.27}$$

Again it is convenient to transform this into an integral over frequency by the use of Parseval's theorem. This yields

$$(1 - P_\infty) \tau_M = \frac{v}{\pi} \Re \int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \frac{d\hat{F}^*(-i\omega)}{d\omega} \hat{G}(-i\omega) d\omega. \tag{2.28}$$

Bound states lead to a divergent contribution to the integral. We return to this point in section 6. The time dependence of the decay may be found from equations (2.18) and (2.21). In the following we derive explicit expressions for the functions $F(t)$ and $G(t)$.

3. Mode analysis

In order to find the time dependence of the decay we must study the analytic properties of the exit amplitude $B(s)$. As noted above, the function has a branch cut along the positive imaginary s axis. There is no singularity at $s = iE_{m_j}$, since the numerator in equation (2.9) vanishes at this point. We define the dispersion function

$$Z(k) = f'_r(c, ivk^2) + ikf_r(c, ivk^2). \quad (3.1)$$

The zeros of $Z(k)$ give rise to singularities in $B(s)$. We write the function $B(s)$ in the form

$$B(ivk^2) = B(0)\Gamma(k), \quad \Gamma(k) = \frac{U(k)}{Z(k)}, \quad (3.2)$$

so that $\Gamma(k)$ has the property $\Gamma(0) = 1$. The denominator $Z(k)$ is independent of the initial wavefunction $\psi(x, 0)$, and is determined by the potential $V(x)$. The numerator $U(k)$ depends on the initial wavefunction. We note that the condition $Z(k) = 0$ can be expressed as

$$\frac{f'_r(c, ivk^2)}{f_r(c, ivk^2)} = -ik. \quad (3.3)$$

This can be interpreted as a matching condition at the exit point $x = c$ between the logarithmic derivative of the regular solution of the Schrödinger equation for $x < c$ and of the outgoing wave $\exp(-ikx)$ for $x > c$. (Recall that we are considering the complex conjugate wavefunction.)

It turns out that in examples the function $\Gamma(k)$ may have branch cuts in the complex k plane, but is analytic about $k = 0$. We may therefore expand as

$$\Gamma(k) = 1 + m_1k + m_2k^2 + m_3k^3 + O(k^4). \quad (3.4)$$

We assume that the potential $V(x)$ is such that the function $\Gamma(k)$ can be written as a sum of simple poles

$$\Gamma(k) = \sum_j \frac{A_j}{k - k_j}. \quad (3.5)$$

In the case of branch cuts the contribution from the cuts takes the form of an integral, which is assumed to be comprised in the above sum. The amplitudes $\{A_j\}$ and poles $\{k_j\}$ satisfy the sum rules

$$\sum_j A_j = 0, \quad \sum_j \frac{A_j}{k_j} = -1, \quad \sum_j \frac{A_j}{k_j^2} = -m_1. \quad (3.6)$$

The first sum rule follows from the fact that $\Gamma(k)$ tends to zero faster than $1/k$ as $k \rightarrow \infty$. The last two follow from equation (3.4). The poles are the complex conjugates of those of the scattering amplitude $S(k)$. Hence bound states correspond to poles on the negative imaginary k axis [15]. There may also be poles on the positive imaginary k axis, as well as conjugate pairs in the upper half of the complex k plane located symmetrically with respect to the imaginary axis. The amplitudes $\{A_j\}$ depend on the initial wavefunction, but the poles $\{k_j\}$ do not. The poles depend only on the potential $V(x)$.

We evaluate the integral by the use of the pole decomposition of $B(-i\omega)$ and the identity

$$\frac{1}{2\pi} \int_{-\infty+i\epsilon}^{\infty+i\epsilon} e^{-i\omega t} \frac{e^{-\alpha x}}{\alpha - q} d\omega = N_0(-iv, q; x, t) \quad (t > 0, v > 0) \quad (3.7)$$

with on the left-hand side $\alpha = \sqrt{\omega/v}$ and complex $q = q' + iq''$ with $q' < 0$. The function on the right-hand side is given by

$$N_0(\mu, q; x, t) = \sqrt{\frac{\mu}{\pi t}} e^{-x^2/4\mu t} + q\mu e^{-qx+\mu q^2 t} \operatorname{erfc}\left(\frac{x}{2\sqrt{\mu t}} - q\sqrt{\mu t}\right). \quad (3.8)$$

The validity of equation (3.7) can be checked by numerical integration. The function $N_0(\mu, q; x, t)$ occurs in item 12 in the table of Laplace transforms in the monograph by Carslaw and Jaeger [12], and can be expressed as

$$N_0(\mu, q; x, t) = \sqrt{\frac{\mu}{\pi t}} e^{-x^2/4\mu t} + q N_1(\mu, q; x, t), \tag{3.9}$$

with the function

$$N_1(\mu, q; x, t) = \mu e^{-qx+\mu q^2 t} \operatorname{erfc}\left(\frac{x}{2\sqrt{\mu t}} - q\sqrt{\mu t}\right). \tag{3.10}$$

The function $N_1(\mu, q; x, t)$ is related to the Moshinsky function [11, 14] $M(k, x, t)$ by

$$N_1(-i, ik; x, t) = -2iM^*(k^*, x, t) \tag{3.11}$$

for real x and t . The notation $N_n(\mu, q; x, t)$ for $n = 0, 1, 2, \dots$ was introduced in work on escape by classical diffusion [12]. The functions of higher order n find application in the problem of escape in three dimensions with centrally symmetric potential and anisotropic initial conditions.

The identity equation (3.7) can be used for those poles k_j which lie in the upper half k plane. For the poles on the negative imaginary axis, corresponding to bound states, we need a modification. For a pole at $-i\kappa$ with $\kappa > 0$, we use the identity

$$\frac{1}{\alpha - \kappa} = \frac{2\kappa}{\alpha^2 - \kappa^2} + \frac{1}{\alpha + \kappa} \tag{3.12}$$

and the corresponding integral

$$\frac{1}{2\pi} \int_{-\infty+i\epsilon}^{\infty+i\epsilon} e^{-i\omega t} \frac{1}{\alpha - \kappa} d\omega = -2i\nu\kappa e^{-i\nu\kappa^2 t} + N_0(-i\nu, -\kappa; 0, t) \quad (\kappa > 0, t > 0). \tag{3.13}$$

We extend this to $x > 0$ in the identity

$$\frac{1}{2\pi} \int_{-\infty+i\epsilon}^{\infty+i\epsilon} e^{-i\omega t} \frac{e^{-\alpha x}}{\alpha - \kappa} d\omega = -2i\nu\kappa e^{-\kappa x - i\nu\kappa^2 t} + N_0(-i\nu, -\kappa; x, t) \quad (\kappa > 0, t > 0). \tag{3.14}$$

It is easily checked that both sides satisfy the conjugate Schrödinger equation in the space $x > 0$. The wavefunction $f(x, t)$ for $x > c$ can be expressed as

$$f(x, t) = f_w(x, t) + f_{os}(x, t) \quad (x > c) \tag{3.15}$$

where the first term is a sum of dispersive waves, and the second is a sum of oscillating terms arising from the bound states. Explicitly, the first term is

$$f_w(x, t) = iB(0) \sum_j A_j N_0(-i\nu, ik_j; x - c, t) \quad (x > c) \tag{3.16}$$

and the second term is

$$f_{os}(x, t) = 2\nu B(0) \sum_{j \in bs} A_j \kappa_j e^{-\kappa_j(x-c) - i\nu\kappa_j^2 t} \quad (x > c) \tag{3.17}$$

where the sum is over the bound states. By using the first sum rule in equations (3.6) and (3.9), the sum over dispersive waves can be simplified to

$$f_w(x, t) = -B(0) \sum_j A_j k_j N_1(-i\nu, ik_j; x - c, t) \quad (x > c). \tag{3.18}$$

At $x = c$, we have

$$N_1(-iv, ik; 0, t) = -iv e^{ivk^2t} \operatorname{erfc}(-ik\sqrt{-ivt}) = -ivw(k\sqrt{-ivt}), \quad (3.19)$$

with the w -function [22] $w(z)$. The value of the derivative is

$$\left. \frac{\partial}{\partial x} N_1(-iv, ik; x - c, t) \right|_{x=c} = -N_0(-iv, ik; 0, t), \quad (3.20)$$

where

$$N_0(-iv, ik; 0, t) = \sqrt{\frac{-iv}{\pi t}} + vkw(k\sqrt{-ivt}). \quad (3.21)$$

Hence the functions $F(t)$ and $G(t)$, defined in equation (2.20), take the form

$$F(t) = F_w(t) + F_{os}(t), \quad G(t) = G_w(t) + G_{os}(t), \quad (3.22)$$

with separate contributions

$$\begin{aligned} F_w(t) &= ivB(0) \sum_j A_j k_j w(k_j \sqrt{-ivt}), & F_{os}(t) &= 2vB(0) \sum_{j \in bs} A_j \kappa_j e^{-iv\kappa_j^2 t}, \\ G_w(t) &= -vB(0) \sum_j A_j k_j^2 w(k_j \sqrt{-ivt}), & G_{os}(t) &= 2vB(0) \sum_{j \in bs} A_j \kappa_j^2 e^{-iv\kappa_j^2 t}. \end{aligned} \quad (3.23)$$

We have again used the first sum rule in equation (3.6). In $F_w(t)$ and $G_w(t)$ the sum is over all modes, including the bound states. The functions have the alternative expressions

$$\begin{aligned} F_w(t) &= iB(0) \sum_j A_j N_0(-iv, ik_j; 0, t), \\ G_w(t) &= -B(0) \sum_j A_j k_j N_0(-iv, ik_j; 0, t), \end{aligned} \quad (3.24)$$

where we have used equation (3.16) and

$$\left. \frac{\partial}{\partial x} N_0(-iv, ik; x, t) \right|_{x=0} = -ikN_0(-iv, ik; 0, t). \quad (3.25)$$

The w -function has the property $w(0) = 1$, whereas the function $N_0(-iv, ik_j; 0, t)$ diverges as $1/\sqrt{t}$ for small t due to the first term in equation (3.21). Nonetheless, the expressions in equation (3.24) are preferable to those in equation (3.23), since for $t > 0$ the sums in equation (3.24) converge faster. It is clear by a comparison with equation (2.35) of García-Calderón *et al* [10] that these authors use an expansion of type (3.23). van Dijk and Nogami [11], in effect, use an expansion of type (3.24).

At large z , the w -function decays as [22]

$$w(z) = \frac{i}{\sqrt{\pi z}} \left[1 + \frac{1}{2z^2} \right] + O\left(\frac{1}{z^5}\right) \quad \left(z \rightarrow \infty, -\frac{5\pi}{4} < \arg z < \frac{\pi}{4} \right). \quad (3.26)$$

The function $N_0(-i, ik; 0, t)$ decays as $t^{-3/2}$ for large t . By using the last two sum rules in equation (3.6), one finds that the coefficient of the leading term in the product $F_w^*(t)G_w(t)$ proportional to t^{-3} is a pure imaginary number times m_1 . By the symmetry properties of the function $\Gamma(k)$ the coefficient m_1 is purely imaginary. Hence in the imaginary part $\Im F_w^*(t)G_w(t)$ the term of order t^{-3} cancels out. As a consequence, the current $J_w(t)$ decays in proportion to t^{-4} , and the corresponding occupancy $P_w(t)$ decays in proportion to t^{-3} .

In principle, in equation (3.16), the wavefunction is decomposed into an infinite sum of running waves. By the choice of the initial wavefunction $\psi(x, 0) = \varphi_{mj}(x)$ the energy spectrum of the outgoing waves, as given by equation (2.25), will be sharply peaked about a resonance energy E_{mj} corresponding to the initial state. We demonstrate this in the following for models which allow a detailed solution.

4. Time-dependent occupancy

In this section, we study the time-dependent occupancy $P(t)$ in more detail. We define a typical timescale for the escape and compare with the mean escape time τ_M . As an illustration we consider a simple model with a potential consisting of a hard wall at $x = 0$, where the wavefunction is required to vanish, and a repulsive delta-function potential $V(x) = (\lambda/a)\delta(x - a)$ located at $a > 0$ of strength $(\lambda/a) > 0$. The model has been studied by Petzold [22], Winter [29], García-Calderón *et al* [10], and van Dijk and Nogami [11].

There are no bound states for this model. As an initial wavefunction $\psi(x, 0)$, we choose

$$\varphi_{m0}(x) = \sqrt{\frac{2}{a}} \Theta(x) \Theta(a - x) \sin \frac{\pi x}{a}, \quad (4.1)$$

where $\Theta(x)$ is the Heaviside step-function, corresponding to the ground state of the particle confined to the interval $0 < x < a$. The ground-state energy is $E_{m0} = v\pi^2/a^2$. The function $f_r(x, s)$ in equation (2.9) is given by

$$\begin{aligned} f_r(x, s) &= \sin kx, & \text{for } 0 < x < a, \\ &= P \sin kx + Q \cos kx, & \text{for } x > a, \end{aligned} \quad (4.2)$$

with coefficients

$$P = 1 + \frac{\lambda}{vka} \sin ka \cos ka, \quad Q = -\frac{\lambda}{vka} \sin^2 ka. \quad (4.3)$$

We take the exit point c just to the right of $x = a$. Then one finds for the exit amplitude $B(s)$ an expression of the form (3.2) with numerator

$$U(k) = \frac{\pi^2(v + \lambda)}{va} \frac{\sin ka}{\pi^2 - k^2 a^2} \quad (4.4)$$

and denominator

$$Z(k) = k \cos ka + \left(\frac{\lambda}{va} + ik \right) \sin ka. \quad (4.5)$$

At $s = 0$

$$B(0) = \frac{i\sqrt{2}}{\pi} \frac{a^{3/2}}{v + \lambda}. \quad (4.6)$$

The expansion coefficient m_1 in equation (3.4) is given by

$$m_1 = -i \frac{va}{v + \lambda}. \quad (4.7)$$

The zeros of $Z(k)$ in the complex k plane are easily found numerically. A complex zero $k_n = k'_n + ik''_n$ is found near $n\pi/a$ for a positive integer n . Its conjugate $k_{nc} = -k'_n + ik''_n = -k_n^*$ is also a zero. The amplitude A_n corresponding to k_n is given by

$$A_n = \left(U(k) \left/ \frac{\partial Z(k)}{\partial k} \right. \right) \Big|_{k=k_n}. \quad (4.8)$$

The amplitude corresponding to k_{nc} is $A_{nc} = -A_n^*$.

The spectral density $g(E)$ is calculated from equation (2.26). We choose units such that $v = 1$ and $a = 1$. In figure 1 we show the spectral density for $\lambda = 10$. It is easily checked numerically that its integral is unity. The spectrum shows a sharp peak near π^2/a^2 . The corresponding root of $Z(k) = 0$ is $k_1 = 2.878 + 0.067i$ and the amplitude A_1 is $A_1 = -1.510 + 0.351i$. Clearly, the poles k_1 and k_{1c} dominate, and as a first approximation to the function $\Gamma(k)$ one can use

$$\Gamma_1(k) = \frac{A_1}{k - k_1} + \frac{A_{1c}}{k - k_{1c}}. \quad (4.9)$$

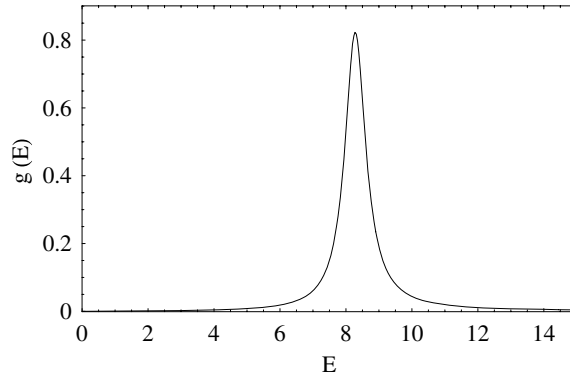


Figure 1. Plot of the energy spectrum $g(E)$ defined in equation (2.26) for the model with delta-function potential with parameters specified below equation (4.8) and initial wavefunction given by equation (4.1).

Similarly, one can include the first n poles up to k_n and the corresponding conjugates up to k_{nc} , and define an approximate function $\Gamma_n(k)$. It is clear that the approximation improves as n increases. For the above numerical example, the plot of the approximate spectral function $g_1(E)$ cannot be distinguished from that of $g(E)$ on the scale of figure 1.

Expression (4.9) gives rise to a factor of the Breit–Wigner form [15], the quantum-mechanical analog of the Lorentz resonance of electromagnetic theory,

$$f_{\text{BW}}(E) = \frac{\gamma_1^2}{(E - E_1)^2 + \gamma_1^2}, \quad (4.10)$$

with resonance energy E_1 and half-width γ_1 given by

$$E_1 = v(k_1^2 - k_1''^2), \quad \gamma_1 = 4vk_1'k_1''. \quad (4.11)$$

Hence one can define the lifetime τ_1 as

$$\tau_1 = \frac{1}{\gamma_1} = \frac{1}{4vk_1'k_1''}. \quad (4.12)$$

The lifetime can be compared with the mean escape time defined in equation (2.16). In this case $P_\infty = 0$. In the integral in equation (2.28), there is a small negative contribution from positive values of the frequency. In figure 2, we compare the rates γ_1 and $\gamma_M = 1/\tau_M$ for the delta-function potential as a function of the strength $L = \lambda/v$. From equation (4.5) one finds by expansion for large L

$$k_1' = \frac{\pi}{a} \left[1 - \frac{1}{L} + \frac{1}{L^2} \right] + O\left(\frac{1}{L^3}\right), \quad k_1'' = \frac{\pi^2}{aL^2} + O\left(\frac{1}{L^3}\right), \quad (4.13)$$

so that with $\lambda = Ka$ the rate γ_1 decreases as

$$\gamma_1 = \frac{4\pi^3 v^3}{K^2 a^4} + O\left(\frac{1}{K^3}\right) \quad (4.14)$$

with increasing strength of the potential. The decrease is only with a power law, not exponential.

The approximate wavefunction corresponding to equation (3.16) and the approximation equation (4.9) is given by

$$f_1(x, t) = iB(0)[A_1 N_0(-iv, ik_1; x - a, t) + A_{1c} N_0(-iv, ik_{1c}; x - a, t)]\Theta(x - a)\Theta(t). \quad (4.15)$$

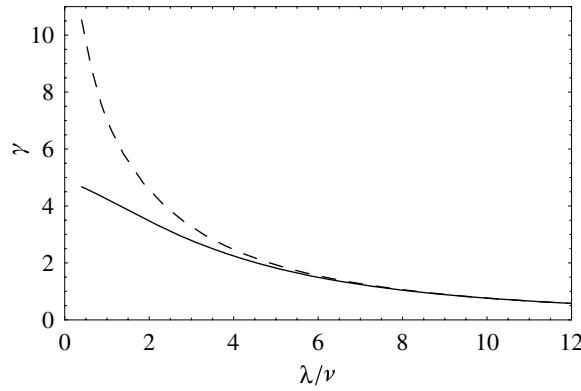


Figure 2. Plot of the mean rate of escape γ_M for the model with delta-function potential as a function of the strength of the potential (solid curve), compared with the rate γ_1 given by equation (4.11) (dashed curve).

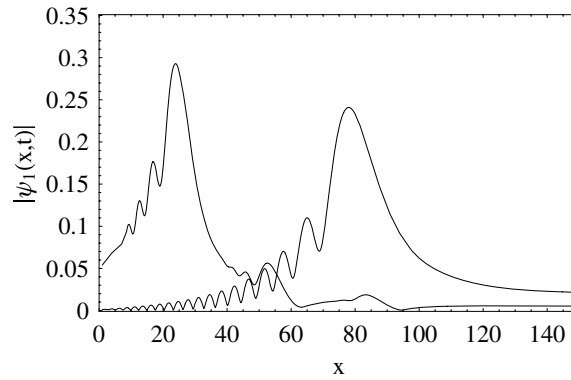


Figure 3. Plot of the absolute value of the approximate wavefunction given by equation (4.15) for the model with parameters specified below equation (4.8) at times $t = 5$ (left peak) and $t = 15$ (right peak).

The wavefunction describes an outgoing wave pulse moving to the right with an approximate speed of k'_1/m . In figure 3, we show the absolute value $|\psi_1(x, t)| = |f_1(x, t)|$ as a function of x at two subsequent times. From equation (3.24), we find the corresponding approximate functions

$$\begin{aligned}
 F_1(t) &= iB(0)[A_1 N_0(-i\nu, ik_1; 0, t) + A_{1c} N_0(-i\nu, ik_{1c}; 0, t)]\Theta(t), \\
 G_1(t) &= -B(0)[A_1 k_1 N_0(-i\nu, ik_1; 0, t) + A_{1c} k_{1c} N_0(-i\nu, ik_{1c}; 0, t)]\Theta(t).
 \end{aligned}
 \tag{4.16}$$

The approximate probability current $J_1(t)$ can be calculated from equation (2.21), and the corresponding occupancy $P_1(t)$ by integration of the current from t to infinity. Higher order corrections can be calculated by including more poles. This leads to small ripples on the wavefunction, but hardly affects the current $J(t)$ or the occupancy $P(t)$. In figure 4 we show the absolute value of the wavefunction in the outer space $x > c$ at time $t = 10$ for the above example, and compare with the value obtained in the first approximation. Similar behavior for $\lambda = 100$ is seen in figure 2 of van Dijk and Nogami [11]. In figure 5 we show

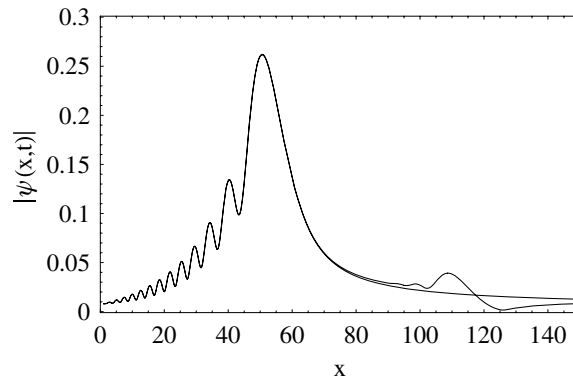


Figure 4. Plot of the absolute value of the wavefunction $\psi(x, t)$ for the model with parameters specified below equation (4.8) at time $t = 10$ compared with that of the approximate wavefunction given by equation (4.15) (smooth curve).

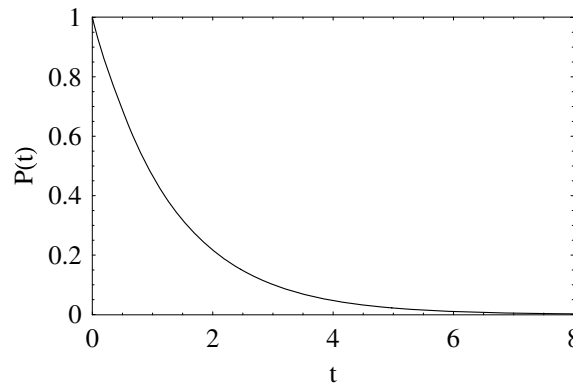


Figure 5. Plot of the occupancy $P(t)$ as a function of t for the same model as in figures 3 and 4.

the corresponding occupancy $P(t)$, which is a smoothly decaying function on the scale of the figure. The first approximation $P_1(t)$ calculated from equation (4.16) cannot be distinguished on the scale of the plot. The ripples seen in figure 5.3 of Razavy [4] are unrealistic, and are due to truncation to only three pairs of terms in a sum of type (3.24).

In the numerical example, the decay time calculated from equation (4.13) is $\tau_1 = 1.306$. The mean escape time τ_M can be calculated from equation (2.27) or from equation (2.28). In the present case $P_\infty = 0$. From equation (2.27) we find $\tau_M = 1.313$, whereas equation (2.28) yields $\tau_M = 1.3146$. The second calculation involves a simple quadrature, and will yield the more accurate result.

In figure 6 we plot $\log|J(t)|$ on a logarithmic timescale. This shows that at long times the current rapidly tends to zero. At long times, when the current is already quite small, it shows oscillations, before finally decaying with a t^{-4} power law. Similar curious behavior of the occupancy $P(t)$ for $\lambda = 6$ was shown in figure 8 of van Dijk and Nogami [11]. In the work of García-Calderón *et al* [10] the occupancy $P(t)$ decayed smoothly, and with an incorrect power law. In a recent work, García-Calderón *et al* [23] have shown that the coefficient of the t^{-3}

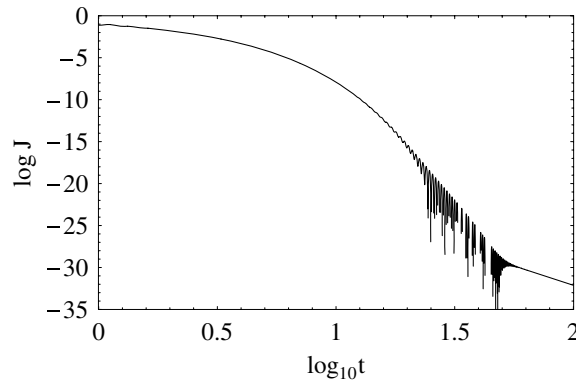


Figure 6. Plot of the logarithm of the probability current $J(t)$ for the same model as in figure 5 as a function of $\log_{10}t$.

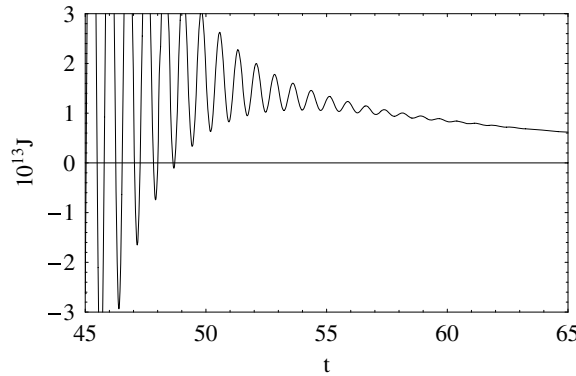


Figure 7. Plot of the probability current $J(t)$ for the same model as in figure 5 as a function of t at long times.

long-time tail in $P(t)$ and in the survival probability $S(t)$ can be found from a steepest-descent calculation. They find good agreement with the calculation from the sum of modes, similar to that performed here.

In order to explain the long-time behavior of the probability current shown in figure 6, we use the first approximation corresponding to the pair k_1, k_{1c} . For example, $J_1(t)$ passes through zero many times in the interval $24 < t < 50$ before finally tending to zero with a positive t^{-4} long-time tail. The actual current $J(t)$, calculated with a larger number of terms, passes through zero many times in the same interval and is numerically close. In figure 7 we show the behavior of $J(t)$ in the time interval $45 < t < 65$. The oscillations in the current before the power law sets in are due to interference of long-time waves, corresponding to the sum of at least two N_0 functions. The waves corresponding to k_1 and k_{1c} run in opposite directions.

If the initial wavefunction is chosen as $\psi(x, 0) = \varphi_{mj}(x)$, instead of the ground state given by equation (4.1), then there will be a corresponding resonance wave number k_{mj} , and similar calculations can be performed. There is an approximate one-line approximation to the spectrum found from the analogue of equation (4.9). Except for the change in complex wave

number the approximate wavefunction has the same structure as in equation (4.15). A linear superposition of such initial states can also be considered.

5. Cut-off parabolic potential

As a second example we consider a cut-off parabolic potential given by

$$V(x) = [V_0 + \frac{1}{2}m\omega_0^2x^2]\Theta(a - x), \quad (5.1)$$

with the cutoff at $a > 0$. For $V_0 < 0$ the potential can have one or more bound states. As initial wavefunction $\psi(x, 0)$ we choose

$$\varphi_{m0}(x) = N_{m0} \exp\left(-\frac{m\omega_0}{2}x^2\right)\Theta(a - x), \quad (5.2)$$

corresponding to the ground state of the particle in the modified potential

$$V_m(x) = V_0 + \frac{1}{2}m\omega_0^2x^2, \quad (5.3)$$

defined for all x . It is convenient to choose units such that $\omega_0 = 1$ and $m = 1$, so that $\nu = \frac{1}{2}$. Then the normalization factor N_{m0} becomes

$$N_{m0} = \frac{\sqrt{2}}{\pi^{1/4}\sqrt{1 + \operatorname{erf}(a)}}. \quad (5.4)$$

The ground-state energy is $E_{m0} = V_0 + \frac{1}{2}$. The function $f_r(x, s)$ in equation (2.9) is given by

$$\begin{aligned} f_r(x, s) &= H\left(\frac{1}{2}k^2 - E_{m0}, -x\right) e^{(a^2-x^2)/2}, & \text{for } -\infty < x < a, \\ &= P \sin kx + Q \cos kx, & \text{for } x > a, \end{aligned} \quad (5.5)$$

where $H(n, x)$ is the Hermite function [24], usually denoted as $H_n(x)$. The coefficients P and Q are found from continuity of the wavefunction and its derivative at $x = a$. We do not need the explicit expressions, since again we take the exit point c just to the right of $x = a$. Then the exit amplitude $B(s)$ takes the form of equation (3.2) with function $Z(k)$ given by

$$Z(k) = (1 + 2V_0 - k^2)H\left(\frac{1}{2}k^2 - \frac{3}{2} - V_0, -a\right) + (ik - a)H\left(\frac{1}{2}k^2 - \frac{1}{2} - V_0, -a\right), \quad (5.6)$$

and function $U(k)$ given by

$$U(k) = Z(0)H\left(\frac{1}{2}k^2 - \frac{3}{2} - V_0, -a\right)/H\left(-\frac{3}{2} - V_0, -a\right). \quad (5.7)$$

At $s = 0$

$$B(0) = 2i e^{-a^2/2} N_{m0} H\left(-\frac{3}{2} - V_0, -a\right)/Z(0). \quad (5.8)$$

The expansion coefficient m_1 in equation (3.4) is given by

$$m_1 = -iH\left(-\frac{1}{2} - V_0, -a\right)/Z(0). \quad (5.9)$$

The zeros of $Z(k)$ in the complex k plane are easily found numerically. For $V_0 \geq 0$ a complex zero $k_n = k'_n + ik''_n$ is found near $\sqrt{2n - 1 + 2V_0}$ for a positive integer n . Its conjugate $k_{nc} = -k'_n + ik''_n = -k_n^*$ is also a zero. The amplitude A_n corresponding to k_n is again given by equation (4.8). The amplitude corresponding to k_{nc} is $A_{nc} = -A_n^*$.

First, we consider the case $V_0 = 0, a = 2$, for which the potential $V(x)$ has no bound states. The numerical value of the smallest zero of $Z(k)$ is $k_1 = 0.989 + 0.020i$. The corresponding amplitude is $A_1 = -0.386 + 0.264i$. For the chosen initial state the poles at k_1 and its conjugate k_{1c} dominate. The spectral density $g(E)$, calculated from equation (2.26), shows a nearly Lorentzian line, centered about $E_1 = 0.488$ and of half-width $\gamma_1 = 0.040$.

The one-line approximation provided by equation (4.9) works again quite well. The spectral line found from the approximate function $g_1(E)$ cannot be distinguished from the exact one on the scale of the plot. The time dependence of the occupancy $P(t)$ is qualitatively the same as for the example in section 4. The lifetime is $\tau_1 = 24.949$, and the mean escape time is $\tau_M = 26.256$. The time dependence of the current is qualitatively the same as before. Between $t = 450$ and $t = 920$ the current passes through zero many times, before finally decaying to zero with a small positive t^{-4} long-time tail. In the time interval $450 < t < 920$, the asymptotic expression (3.26) is not yet adequate for the smallest zero k_1 .

We compare with the approximate expressions for the energy E_1 and the half-width γ_1 derived by Gurvitz *et al* [30, 19]. Taking the separation distance R in their two-potential approach at $a = 2$ we find from equations (9) and (10) in [19] the approximate values $E_1 = 0.481$ and $\gamma_1 = 0.036$, fairly close to the exact values $E_1 = 0.488$ and $\gamma_1 = 0.040$ found above. The modified two-potential approach of [19] with $G_k(x) = \cos kx$ and $\bar{r} = 2$ in their equation (16) yields the improved value $E_1 = 0.490$. The last factor in equation (16) cannot be replaced by unity. For this example their equation (23) is not a good approximation to the half-width in equation (9).

Using identities derived elsewhere [25] one can show that for $V_0 = 0$ the asymptotic behavior of the zero k_1 for large a is given by

$$k_1 \approx 1 - \frac{a}{\sqrt{\pi}} e^{-a^2} + \frac{2i}{\sqrt{\pi}} e^{-a^2} \quad (V_0 = 0, \text{ as } a \rightarrow \infty). \quad (5.10)$$

This implies that asymptotically the rate γ_1 is given by

$$\gamma_1 \approx \frac{4}{\sqrt{\pi}} e^{-a^2} = \frac{4}{\sqrt{\pi}} e^{-2V(a)} \quad (V_0 = 0, \text{ as } a \rightarrow \infty). \quad (5.11)$$

Gamow's expression for the lifetime [3], based on a WKB-argument, yields for the present case

$$\gamma_G \approx 8 e^{-2V(a)} \quad (V_0 = 0, \text{ as } a \rightarrow \infty). \quad (5.12)$$

This differs in the prefactor from equation (5.11), and overestimates the actual rate by a factor of 3.54.

Next we consider the case $V_0 = -1, a = 2$. In this case there is a single bound state at $E_0 = -0.507$, corresponding to the zero $k_b = -1.007i$ of the function $Z(k)$. The amplitude of the pole is $A_b = 0.235i$. There is a corresponding zero at $k_{bc} = 1.122i$ with amplitude $-1.366i$. The pair nearest to the origin of the complex k plane is at $k_1 = 0.949 + 0.157i$ and $k_{1c} = -k_1^*$ with amplitudes $A_1 = 0.035 + 0.088i$ and $A_{1c} = -A_1^*$. For the bound state corresponding to $k_b = -i\kappa_b$, the wavefunction for $x > a$ decays exponentially as $Q_b \exp(-\kappa_b x)$. For $x < a$ it is given by

$$\varphi_0(x) = N_0 H\left(\frac{1}{2}k_b^2 + \frac{1}{2}, -x\right) e^{-x^2/2}. \quad (5.13)$$

The coefficient Q_b is evaluated from the conditions of continuity of the wavefunction and its derivative at $a = 2$. This yields $Q_b = 1.433$. Using this one finds for the normalization constant $N_0 = 0.742$. The probability P_∞ of remaining in the bound state is calculated as the square of the overlap integral

$$I_{00} = \int_{-\infty}^a \varphi_0(x) \varphi_{m0}(x) dx. \quad (5.14)$$

This yields $P_\infty = 0.989$. The probability of escape is therefore quite small. The spectrum of emitted waves $g(E)$, as calculated from equation (2.26), is shown in figure 8. An approximation $\Gamma_2(k)$ to the function $\Gamma(k)$ can be evaluated from the four dominant poles

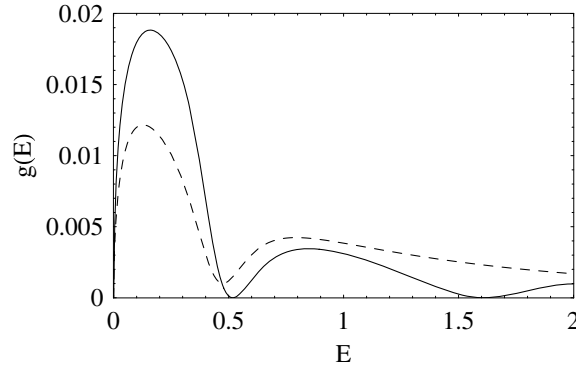


Figure 8. Plot of the energy spectrum $g(E)$ for the model with parabolic potential with cutoff at $a = 2$ and potential minimum $V_0 = -1$ for decay from the ground state at energy $E_{m0} = -\frac{1}{2}$ (solid curve) compared with that calculated from the approximation with four dominant poles (dashed curve).

listed above. The agreement of the spectral function $g_2(E)$ with the exact spectrum $g(E)$ at small E is only modest, as shown also in figure 8, but at higher values of E it provides a smooth interpolation through the many peaks of $g(E)$. The time-dependent occupancy $P(t)$, as well as the approximation $P_2(t)$ to this function corresponding to the dominant poles, can be calculated as before.

Finally, we change the initial state to the first excited state

$$\varphi_{m1}(x) = N_{m1} x e^{-x^2/2} \Theta(a - x), \quad (5.15)$$

with the normalization factor N_{m1} . The function $U(k)$ changes to

$$U(k) = Z(0) \frac{3 + 2V_0}{k^2 - 3 - 2V_0} \frac{a(k^2 - 1 - 2V_0)H\left(\frac{1}{2}k^2 - \frac{3}{2} - V_0, -a\right) + H\left(\frac{1}{2}k^2 - \frac{1}{2} - V_0, -a\right)}{a(1 + 2V_0)H\left(-\frac{3}{2} - V_0, -a\right) - H\left(-\frac{1}{2} - V_0, -a\right)}. \quad (5.16)$$

The value $B(0)$ becomes

$$B(0) = 2i e^{-a^2/2} N_{m1} \frac{a(1 + 2V_0)H\left(-\frac{3}{2} - V_0, -a\right) - H\left(-\frac{1}{2} - V_0, -a\right)}{(3 + 2V_0)Z(0)}. \quad (5.17)$$

The positions of the poles are the same as before, but the amplitudes change. We consider the potential with $V_0 = -1$, $a = 2$. For the bound state amplitude one now finds $A_b = -0.001i$, for the amplitude of the pole at k_{bc} one finds $A_{bc} = 0.157i$ and for the amplitude of the pole at k_1 one finds $A_1 = -0.404 + 0.359i$. From the overlap integral I_{01} , defined in analogy to equation (5.14), one finds that the probability of remaining in the bound state $\varphi_0(x)$ is only $P_\infty = 0.0001$. The emission spectrum shows a fairly broad peak near $E = 0.5$. In figure 9 we show the spectrum $g(E)$, as calculated from equation (2.26), as well as the approximate spectral function $g_2(E)$ calculated from the four dominant poles. The lifetime is $\tau_1 = 3.351$. As noted at the end of section 2, the mean escape time given by equation (2.28) diverges if there is a bound state. In the following section we define a modified mean escape time which is finite.

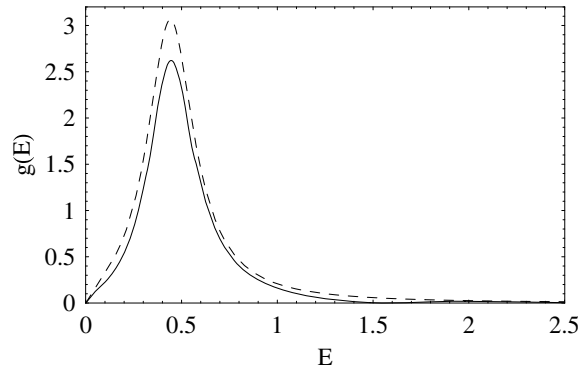


Figure 9. Plot of the energy spectrum $g(E)$ for the model with parabolic potential with cutoff at $a = 2$ and potential minimum $V_0 = -1$ for decay from the first excited state at energy $E_{m1} = \frac{1}{2}$ (solid curve) compared with that calculated from the approximation with four dominant poles (dashed curve).

6. Solution for all time

It is clear from a comparison of equation (2.14) with equation (9) of van Dijk and Nogami [11] that the two solutions differ. In case there are no bound states, then the wavefunction $\psi(x, t)$, when written as a superposition of stationary states, involves time factors $\exp(-i\omega t)$ with only positive frequencies ω , corresponding to positive energy. Our expression for $\psi(x, t) = f^*(x, t)$ involves negative as well as positive frequencies. It is evident from equation (2.14) that the negative frequencies correspond to non-propagating waves. Both solutions to the problem must be identical for $t > 0$. The solution in equation (9) of van Dijk and Nogami is also valid for $t < 0$. It contains incoming waves which build up the wavefunction to its value at $t = 0$. We have solved the initial-value problem for the given wavefunction $\psi(x, 0)$ at $t = 0$ by the method of Laplace transform, and our solution vanishes identically for $t < 0$.

The relation between the two solutions is therefore clear. If we define the Fourier transform of the wavefunction by

$$\Psi(x, \omega) = \int_{-\infty}^{\infty} \psi(x, t) e^{i\omega t} dt, \tag{6.1}$$

then it can be decomposed [21, 26] into a ‘positive-frequency part’ $\Psi_+(x, \omega)$ and a ‘negative-frequency part’ $\Psi_-(x, \omega)$,

$$\Psi(x, \omega) = \Psi_+(x, \omega) + \Psi_-(x, \omega), \tag{6.2}$$

defined by [2, 4]

$$\Psi_+(x, \omega) = \int_0^{\infty} \psi(x, t) e^{i\omega t} dt, \quad \Psi_-(x, \omega) = \int_{-\infty}^0 \psi(x, t) e^{i\omega t} dt. \tag{6.3}$$

The positive-frequency part $\Psi_+(x, \omega)$ suffices to reconstruct the solution $\psi(x, t)$ for $t > 0$ by an inverse Fourier transform. Our solution is just the positive-frequency part of the solution in equation (9) of van Dijk and Nogami, and corresponds to their equation (16), which holds only for $t > 0$. The solution simplifies because information which is superfluous for $t > 0$ is discarded. The function $\Psi_+(x, \omega)$ is analytic in the upper half of the complex ω plane. This corresponds to the right half of the complex s plane, since $s = -i\omega$. Explicitly,

$$\Psi_+^*(x, \omega) = \hat{f}(x, i\omega^*). \tag{6.4}$$

Since we have chosen $\psi(x, 0)$ to be real, the wavefunction for $t < 0$ can be obtained from that for $t > 0$ by the relation

$$\psi(x, -t) = \psi^*(x, t). \quad (6.5)$$

The relation implicitly assumes that the wavefunction at $t = 0$ is built up by incoming waves. What is observed by a detector in the outer space should be calculated from the wavefunction for $x > c$ and $t > 0$, as given by equation (2.14).

Our solution $f(x, t) = \psi^*(x, t)$ for $t > 0$ involves for $x > c$ a continuum of waves propagating to the right, a continuum of non-propagating solutions and a discrete set of oscillatory bound solutions. Since we consider the conjugate wavefunction, the propagating solutions correspond to negative frequency, or positive energy, the other ones to positive frequency, or negative energy. We can make the separation explicit by writing

$$f(x, t) = f_p(x, t) + f_n(x, t), \quad (6.6)$$

where by comparison with equation (2.14)

$$\begin{aligned} f_p(x, t) &= \frac{1}{2\pi} \int_{-\infty+i\epsilon}^{0+i\epsilon} B(-i\omega) e^{-ik(x-c)-i\omega t} d\omega, \\ f_n(x, t) &= \frac{1}{2\pi} \int_{0+i\epsilon}^{\infty+i\epsilon} B(-i\omega) e^{-ik(x-c)-i\omega t} d\omega \quad (x > c). \end{aligned} \quad (6.7)$$

The poles of $B(-i\omega)$ for positive ω give rise to the bound state contributions to $f_n(x, t)$. The remainder of $f_n(x, t)$ is a transient decaying to zero by dispersion.

We define functions $F_p(t)$, $F_n(t)$ and $G_p(t)$, $G_n(t)$ from the analogue of equation (2.20). The part of the probability current corresponding to propagating waves is then given by

$$J_{pp}(t) = 2v \Im F_p^*(t) G_p(t). \quad (6.8)$$

This will correspond to the pulse seen by a detector at some distance from the source. In analogy to equation (2.28) the mean escape time for the pulse is defined by

$$(1 - P_\infty) \tau_{Mp} = \frac{v}{\pi} \Re \int_{-\infty+i\epsilon}^{0+i\epsilon} \frac{d\hat{F}^*(-i\omega)}{d\omega} \hat{G}(-i\omega) d\omega. \quad (6.9)$$

For the example with the delta-function potential treated in section 4 this takes the value $\tau_{Mp} = 1.3150$, almost the same as $\tau_M = 1.3146$. For the first excited state decaying and escaping from the parabolic potential treated at the end of section 5 the value is $\tau_{Mp} = 5.195$. This is substantially larger than $\tau_1 = 3.351$ on account of the broad spectrum.

7. Discussion

The Laplace transform of the time-dependent wavefunction for the models studied has a concise form, and leads naturally to a decomposition of the wavefunction into a sum of wave modes and bound states. We have shown in the last section that the sum of wave modes itself can be decomposed into a propagating and a non-propagating part. The wavefunction in the outer space is found in an explicit form, which is the same for all potentials. This suggests that in a numerical solution of the Schrödinger equation [27, 28] it may be sufficient to restrict attention to the inner space.

As initial wavefunction we have chosen one of the eigenfunctions $\{\varphi_{mj}(x)\}$ for the modified confining potential $V_m(x)$. One can also consider a linear superposition of such states. This would correspond to a linear superposition of expressions of the form (2.10) for the exit amplitude. The dispersion function $Z(k)$ in the denominator is common to all

expressions, and only the numerator of the amplitude would change. A thermal ensemble of initial states would lead to an averaged expression with the same denominator. At higher temperatures a large number of zeros of the denominator contribute, and an effective method is needed to discuss the mechanism of escape corresponding to the averaged expression. It would be of interest to compare such a calculation with the theory of stimulated quantum tunneling in the presence of dissipation and random forces.

The present analysis of spontaneous quantum tunneling can be carried through straightforwardly for model systems with simple potentials, for example a parabolic well followed by a parabolic barrier, followed by open space. Since analytic expressions are obtained, the effect of a change in the parameters is easily explored. It would be of interest to investigate the effect of the shape and height of the barrier on the time dependence of escape, in analogy to the theory of escape by classical diffusion [25].

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