Universal potential barrier penetration by initially confined wavepackets

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PACS numbers: 03.65.-w, 03.65.Nk, 03.65.Xp.

Introduction The tunneling phenomenon is a fundamental problem in quantum mechanics. Traditionally, it is solved and presented in most textbooks for a particle with a given energy and momentum (see, for example [1]). Although this treatment is usually sufficient to demonstrate the main features of tunneling, it raises a serious difficulty, for the uncertainty principle suggests that the particle is instantaneously distributed over the entire space. Clearly, this analysis implies that the particle was and always will be at both sides of the barrier, and therefore the classical meaning of tunneling is not clear. This problem is one of the reasons that researchers investigated the dynamics of wavepackets, usually Gaussians, in the process of tunneling [2]. Although this treatment seems more intuitive, whenever the initial wavepacket is analytic there is always initially a tail at the other side of the barrier. To prevent this problem, the initial wavepacket must be singular and to have a non-zero value only at a finite region in space.

Clearly, tunneling is just one specific case in a much broader family of scattering problems, and all that was said above can be generalized to transmission through any arbitrary potential.

During the last few years, due to the recent development in femto-second pulses lasers [3, 4], optical tweezers and atom cooling and trapping [5, 6], an interest in Moshinsky’s shutter problem [7] was rejuvenated [8, 9, 10, 11, 12]. Moshinsky was the first to investigate the dynamics of an initially singular wavefunction. The singularity of the initial wavefunction modeled a fast shutter. The ability to localize particles (usually atoms) by laser beams and then to release them instantaneously increases the feasibility to simulate the shutter [12, 14].

In this paper we derive a generic formula for the Schrödinger dynamics of an initially singular wavefunction (which vanishes at half space) in the presence of a finite-width potential.

It should be stressed that even if the initial wavefunction is a smooth function (rather than singular) with a transition length scale of ε, then the results presented here are valid provided the measurements are done at distances shorter than $t_h/2m\varepsilon$ (see ref. [11]).

The general case A wavefunction is confined to one side of a potential barrier. The barrier is located around $L > 0$ and vanishes for $x < 0$ and $x \rightarrow \infty$. The initial wavepacket, on the other hand, vanishes beyond $x > 0$ (see Fig.1). Therefore, initially, there is no overlap between the wavepacket and the barrier. The dynamics are governed by the Schrödinger equation

$$- \frac{\partial^2}{\partial x^2} \psi + V(x - L) \psi = \frac{\partial \psi}{\partial t},$$  

where $V(x)$ is the potential barrier. Hereinafter, the units $\hbar = 1$ and $2m = 1$ are used.

Since the initial wavefunction has a singularity at $x = 0$ it can be written as

$$\psi(x, t = 0) = f(x) \theta(-x),$$

and the solution at $t > 0$ and $x > L$ is then

$$\psi(x, t) = \int \frac{dk dq}{2\pi} F(q) \frac{iT(k)}{k - q + i0} \exp(ikx - ik^2t).$$

In this equation $F(q) \equiv (2\pi)^{-1} \int dx f(x) \exp(-iqx)$ is the Fourier transform of $f(x)$ and $T(k)$ is the transmission coefficient of the barrier for plane-wave with momentum $k$.

The properties of the barrier and the initial wavefunction can be separated by defining

$$\varphi(q, x, t) \equiv \frac{1}{2\pi} \int \frac{dk}{k - q + i0} \exp(ikx - ik^2t),$$
and hence

\[ \psi(x, t) = \int dq \varphi(q, x, t) F(q), \quad (4) \]

which, by expanding \( \varphi(q, x, t) \) in orders of \( q \), Eq. (4) can be rewritten in terms of \( f(x) \). We thus obtain the generic solution of the problem:

\[ \psi(x, t) = \varphi \left( -i \frac{\partial}{\partial \xi}, x, t \right) f(\xi) \bigg|_{\xi=0}. \quad (5) \]

This generic expression should be interpreted as the infinite expansion

\[ \psi(x, t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \frac{\partial^n}{\partial q^n} \varphi(q, x, t) \big|_{q=0} \frac{\partial^n}{\partial \xi^n} f(\xi) \bigg|_{\xi=0} = \varphi(0, x, t) f(0) - i \varphi'(0, x, t) f'(0) + \cdots, \quad (6) \]

where \( \varphi'(0, x, t) \equiv \partial \varphi(q, x, t) / \partial q \big|_{q=0} \) and \( f'(0) \equiv \partial f(x) / \partial x \big|_{x=0} \).

Eqs. (4) and (5) are the main result of this paper. It is evident from Eq. (6) that the wavefunction dynamics depend only on the initial wavepacket values at the boundary \( x = 0 \). It is a universal formula in the sense that any wavefunction \( f(x) \) and any potential can be substituted in it to find the exact dynamics beyond the potential at any \( t > 0 \). In particular, when \( f(x) = C \) is a constant, then the solution is simply

\[ \psi(x, t) = C \varphi(0, x, t). \quad (7) \]

Eq. (4) can also be written as the following expansion

\[ \psi(x, t) = \sum_{n=0}^{\infty} a_n f^{(n)}(0), \quad (8) \]

where \( f^{(n)}(0) \equiv \partial^n f(\xi) / \partial \xi^n \bigg|_{\xi=0} \) are the initial function’s derivatives and the coefficients are

\[ a_n = \frac{s^{n+1}}{2\pi n!} \int dk \frac{T(k)}{(k + i0)^{n+1}} \exp(ikx - ik^2t). \quad (9) \]

These coefficients can be written also as an expansion by expanding \( T(k) / (k + i0)^{n+1} \) around the momentum \( x/2t \) (the dominant term in the stationary phase approximation in long times and arbitrary \( x \)), i.e.,

\[ T(k) = \frac{\partial^n [T(q) / q^{n+1}] }{\partial q^{n+1} } \bigg|_{q=x/2t} \quad (10) \]

By substituting Eq. (10) in Eq. (9) and Eq. (8) one obtains

\[ \psi(x, t) = \frac{1}{2\pi} \exp \left( \frac{x^2}{4t} \right) \sum_{n=0}^{\infty} b_n f^{(n)}(0), \quad (11) \]

where the coefficients are

\[ b_n = \frac{i^{n+1}}{n!} \sum_{m=0}^{\infty} s_{n,2m} \frac{1}{(2m)!} \left( m + \frac{i}{2} \right) \left( it \right)^{-(2m+1)/2}, \quad (12) \]

and \( s_{n,2m} \equiv \frac{\partial^{2m}}{\partial q^{2m}} \left[ T(k) k^{-n-1} \right]_{k=x/2t} \). This result also suggests that at large distances \( x^2 / t \to \infty \)

\[ \psi(x, t) \sim T \left( \frac{x}{2t} \right) \frac{i^{n+1}}{2^{m+1} \pi} \frac{e^{ix^2/4t}}{x} f(0), \quad (13) \]

and the particles density decays like \( \rho = |\psi(x, t)|^2 \sim [T(x/2t) f(0)]^2 tx^{-2}/\pi \), which agrees with the free results [11] for \( T = 1 \). Moreover, for every finite potential \( T(k \to 0) \to 1 \), which means that at very short times (with respect to the distance, i.e., \( t/x^2 \ll 1 \), although it was derived for large \( t \)) Eq. (13) is reduced to the free propagation for every potential, which is consistent with [12].

Specific examples and applications In this section we will demonstrate these derivations in a few scenarios for different potentials.

The delta function potential – an exact solution

One of the simplest scenarios of a potential barrier penetration is the delta-function potential (see Fig.2A). This problem was discussed in detail for an initially singular...
wave function in [12], and is presented here only to illustrate the validity of the above derivations. In this case the Schrödinger equation reads: 

\[ \psi(x > L, t) = \frac{e^{ix^2/4t}}{2} \left\{ \frac{\partial}{\partial x} \left( \frac{x}{2t} + i \frac{\partial}{\partial \xi} \right) - \frac{\lambda/2}{\partial/\partial \xi + \lambda/2} \right\} f(\xi)|_{\xi=0}. \]  

This expression obviously agrees with [12], and illustrates the fact that the dynamics are fully described by the values of the initial wavefunction at the singular point.

At short times, i.e., \( t << x^2 \), it can be expanded (see [12])

\[ \psi(x, t) \cong \sqrt{\frac{it}{\pi}} \frac{e^{ix^2/4t}}{x} \left[ f(0) + O(x^{-2}) \right]. \]  

That is, in the leading terms, the influence of the barrier was eliminated by changing the derivative of the initial wavefunction only at the singularity point for \( \sqrt{t}/x \ll 1 \). In general, each one of the terms in the expansion can be eliminated (except for the first one) by tailoring the derivatives of the wavefunction at the singular point.

The rectangular potential barrier. In the case of the rectangular potential barrier (see Fig. 2C), with potential

\[ -\frac{\partial^2}{\partial x^2} \psi - 2a^2 \text{sech}^2 [a(x - L)] \psi = i \frac{\partial \psi}{\partial t} \]  

The transmission coefficient in this case is well known \( T(k) = k/(k - i\lambda/2) \), in which case by Eqs. 14 and 15 the solution beyond the barrier is

\[ T(k) = \frac{\exp(-2ikL)}{\cosh(2\kappa L) + i(\epsilon/2) \sinh(2\kappa L)}, \]  

where \( \kappa \equiv \sqrt{V_0 - k^2} \) and \( \epsilon \equiv k/L - k/k_\text{bar}. \) At short times, the particles that penetrate the barrier are extremely energetic and therefore they pass the barrier almost unaffected by it.

In this case \( \kappa \equiv ix/2t, \epsilon \equiv i \left[ 1 + 2(V_0t^2/x^2)^2 \right] \) and

\[ T \left( \frac{x}{2t} \right) \cong \left[ 1 - 2i(V_0t^2/x^2)^2 \sin(xL/t) \exp(i xL/t) \right]^{-1}, \]  

which yields by Eq. 18

\[ \psi(x, t) \rightarrow \frac{e^{ix^2/4t} f(0) \sqrt{it/\pi}}{1 - 2i(V_0t^2/x^2)^2 \sin(xL/t) e^{ixL/t}}, \]  

with weak resonances at \( xL/t = m\pi \), (where \( m \) is an integer).

A Reflectionless potential. One of the peculiar potential examples is the reflectionless potential [17, 15]. For this potential (see Fig. 2D) the absolute value of the transmission coefficient is always \( |T(k)| = 1 \). Therefore, the reflection coefficient is zero for every incoming plane wave; however, the transmission coefficient suffers from dispersion, which deforms the initial wavepacket. It is well known that the potential \( V(x) = -2a^2 \text{sech}^2(ax) \), whose width goes like \( \sim a^{-1} \) and its depth like \( a^2 \), belongs to a family of reflectionless potentials [12, 16, 17].

This potential, as opposed to the previous three, is not completely localized in space. That is, the initial wavefunction "feels" the potential at any distance. Therefore, one should place it at a large distance from the edge of the initial wavefunction. Its Schrödinger equation is then

\[ -\frac{\partial^2}{\partial x^2} \psi - 2a^2 \text{sech}^2 [a(x - L)] \psi = i \frac{\partial \psi}{\partial t}, \]  

where \( L \gg a^{-1} \) is the new location of the potential well. This equation has an exact reflectionless solution (which
corresponds to the incoming plane wave $\psi(x \to -\infty) \sim \exp(ikx) + R(k) \exp(-ikx)$)

$$\psi(x) = [k/a + i \tanh(ax)](k/a - i)^{-1} \exp(ikx). \quad (21)$$

For $x \to \infty$ Eq. (21) can be written $\psi(x) \sim T(k) \exp(ikx)$ with the simple transmission coefficient $T(k) = \frac{k + ia}{k - ia}$. According to Eqs. (23),

$$\varphi(q, x > L, t) = \frac{1}{2\pi} \int \frac{dk}{k - q + ia} \exp(ikx - ik^2 t),$$

which can easily be written as

$$\varphi(q, x, t) = \varphi_{\text{free}}(q, x, t) - 2a \frac{q}{q - ia} \left[ \varphi_{\text{free}}(q, x, t) - \varphi_{\text{free}}(a, x, t) \right], \quad (22)$$

where $\varphi_{\text{free}}(q, x, t)$ is the free (without the barrier) solution $\varphi_{\text{free}}(q, x, t) = \frac{1}{\sqrt{2\pi}} \exp\left( \frac{q^2}{2t} \right)$.

Again, at short times $t << x/a$ the free solution is retrieved (the two expressions on the right cancel each other).

Conclusions and summary

We have presented a generic formula, which describes the solution of the temporal propagation through an arbitrary potential of an initially singular wavefunction. It was shown that when the initial wavefunction vanishes at the entire half space, i.e., $\psi(x, t = 0) = f(x) \theta(-x)$ the wavefunction for every $t$ is $\psi(x, t) = \varphi(-i \frac{\partial}{\partial \xi}, x, t) f(\xi)$.

Particularly, it is shown that at very large distances the solution can be approximated by the generic expression for any initial function $\psi(x, t = 0) = f(x) \theta(-x)$ the general solution is $\psi(x, t) \sim T(x) \sqrt{\frac{e^{ix^2/At}}{\pi}} f(0)$. The authors are indebted to Miriam Schler for her networking efforts.

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