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Short-time quantum dynamics of sharp boundaries potentials

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ABSTRACT

Despite the high prevalence of singular potential in general, and rectangular potentials in particular, in applied scattering models, to date little is known about their short time effects. The reason is that singular potentials cause a mixture of complicated local as well as non-local effects.

The object of this work is to derive a generic method to calculate analytically the short-time impact of any singular potential.

In this paper it is shown that the scattering of a smooth wavefunction on a singular potential is totally equivalent, in the short-time regime, to the free propagation of a singular wavefunction. However, the latter problem was totally addressed analytically in Ref. [7]. Therefore, this equivalency can be utilized in solving analytically the short time dynamics of any smooth wavefunction at the presence of a singular potentials. In particular, with this method the short-time dynamics of any problem where a sharp boundaries potential (e.g., a rectangular barrier) is turned on instantaneously can easily be solved analytically.

1. Introduction and motivation

Due to recent advances in Scanning Tunneling Microscopy (STM) [1–3] and optical tweezers [4,5] technologies, it became feasible to turn on and off quantum potentials almost instantaneously. Moreover, these dynamic potentials (especially STM's) can have very sharp boundaries (compared to the particles' wavelength), and therefore can be regarded, with high accuracy, as singular potentials (e.g., rectangular, or delta potentials). Rapid changes in potentials and quantum barriers can be used in numerous scenarios (see, for example Ref. [6]) but especially in fast nanoelectronics.

Despite the fact that it is well known that singular initial conditions create nonlocal effects in the short time [7], there is currently no general analytical theory or method to evaluate the short time quantum effect of singular potentials.

Usually, the problem is circumvented by using three approaches. One option is to approximate the problem as a stationary one. Most applied quantum tunneling models are based on continuous waves with stationary barriers, in which cases the quantum entity has a well-defined energy and momentum, but its location is spread over the entire space(e.g. [8,9]).

The second option is to assume that initially there is no overlap between the initial wavefunction and the potential (usually barrier). This is possible only if both of them (the wavefunction and the potential) are singular since they both must vanish on, at least, finite intervals. This approach was taken in previous publications [10,11,12,13].

Motivated by the generic behavior of initially singular wavefunction [7], we have shown that a generic solution can be derived for a singular wavefunction in the presence of any potential (not necessarily a barrier).

It may seem that taking initially a singular wavefunction is not a physical assumption (although it is fully consistent with the Schrödinger dynamics and actually essential for the completeness of the Hilbert space), and indeed, whenever this problem is encountered in the literature a smooth wavefunction is used, albeit the solution is based on the continuous wave approach [8,9]. That is, the initial wavepacket is dismantled into its spectral components, which are then reassembled again after multiplying each one of them by the relevant transfer function.

Mathematically, a correct approach would be to disassemble the initial smooth wavefunction $\psi(x)$ to the eigenstate of the potential (which can have singular boundaries) $\chi_k^{\pm}(x)$, i.e.,

$$\psi(x) = \int \left[a_k^+ \chi_k^+(x) + a_k^- \chi_k^-(x)\right] dk. \tag{1}$$

The temporal dynamics is then trivial

$$\psi(x, t) = \int \left[a_k^+ \chi_k^+(x) + a_k^- \chi_k^-(x)\right] \exp(-ik^2 t) dk. \tag{2}$$

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The problem with this approach is that the eigensatates $\chi_k(x)$ are complicated functions (and are not analytical in the case of a potential with singular boundaries) and therefore finding the coefficients a_k is a difficult task. Another option is to use the Kernel of a step function potential, but as can be seen from Refs. [14,15] this approach is very complicated.

To make the calculations easier an intuitive method is taken, where the initial wavepacket is located on one side of the potential [16], i.e. it is assumed, erroneously, that there is no overlap between the initial wavepacket and the barrier. In this case the problem is reduced to a simple Fourier analysis

$$\psi(x) = (2\pi)^{-1} \int a_k \exp(ikx)dk. \tag{3}$$

However, this approach bypasses the problem rather than confront it, because initially there is an overlap between the two. Moreover, initially there is always some part of the wavefunction beyond the potential.

The legitimacy of using this approach can be based on numerical simulations, which indeed back it up [17]. However, the consistency between the two appears due to the fact that usually there is initially a negligible overlap between the wavefunction and the potential, and if the overlap is not negligible then it takes time for the consistency to appear, when most of the wavepacket already "passed through" the barrier (if a classical-particle terminology can be adopted). So, in fact, the interesting short-time effect is missing.

Currently, despite the fact that singular (or, at least, sharp boundaries) potentials are most commonly used in the literature for applied quantum mechanics models, and although singular potentials have a large non-local effect in the short time, there is no generic theory for calculating their effect on the wavefunction in the short time.

Usually, every scenario is treated differently, and therefore it is very difficult to identify the common general physics of the short time impact of singular potentials.

In previous works we formulated the generic short-time dynamics of singular wavefunctions with continuous potential [10] and singular wavefunctions with singular potential, where initially there is no overlap between the two [11] (Fig. 1a).

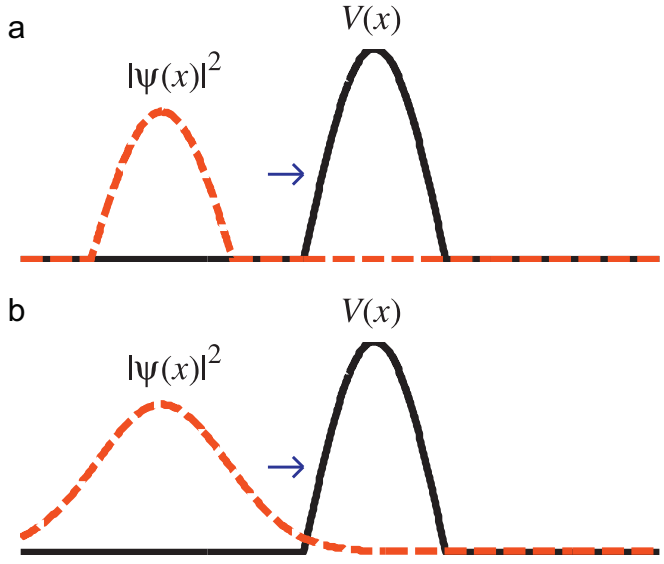

Fig. 1. Scattering scenarios: (a) no overlap between the initial wavepacket (dashed lcurve) and the potential barrier (solid curve); (b) there is an overlap between the initial wavefunction (dashed curve) and the potential barrier (solid curve).

In order to investigate the short-time influence of singular potentials on smooth wavefunctions (Fig. 1b) we need a different approach.

Physically, this mathematical description is equivalent for turning on the potential instantaneously, where the initial smooth wavefunction is already present.

The problem here is, that unlike the case where the wavefunction is singular (and the potential is arbitrary), in the present case we cannot use the simple Kernel of the free-propagation Schrödinger dynamics. The potential is introduced in the kernel in a non-trivial way (see Refs. [14,15]), and unlike the smooth potential case, cannot be ignored. In the case where the wavefunction is singular, the presence of the potential (singular or not) can be ignored (it is explained in Ref. [10]), however, if the initial wavefunction is smooth – the potential cannot be disregarded, and evidently neither can its singularities (if exist).

2. Theory

Let us assume that the potential is not really singular but rather smooth with very sharp transitions (high values derivatives). This is a legitimate assumption since most realistic problems are indeed smooth, and we will see that this assumption is consistent with the result (see also Ref. [7]).

With this assumption in hand, the wavefunction is differentiable and one can use the ordinary Schrödinger equation dynamics, i.e.

$$i\frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2} + V(x)\psi \tag{4}$$

where the units $\hbar = 1$ (reduced Planck constant) and $2m = 1$ (particle's mass) were adopted.

Clearly, the temporal change in the wavefunction (the left hand term of the equation) depends merely on the Hamiltonian operation on the wavefunction. This is an important point and should be stressed. The cause of the singularity is not essential. Its consequence will be identical provided the right hand side of the equation is the same.

Suppose that $V(x)$ is a singular potential, i.e., without loss of generality, at $x = 0$, there is a certain singularity in $V(x)$. Let $\psi_A(x)$ be the initial analytical function. In this case, one can define a different wavefunction$\psi_S(x)$ that satisfies

$$-\frac{\partial^2\psi_S}{\partial x^2} \equiv -\frac{\partial^2\psi_A}{\partial x^2} + V(x)\psi_A \tag{5}$$

In this case the initial temporal change of both functions will be exactly the same.

Therefore, the instantaneous temporal change (after turning on the potential) of the smooth function (with singular potential) is exactly equal to the temporal change of an equivalent singular wavefunction $\psi_S(x)$ that satisfies (5).

Since we are interested in the short time regime, and since $\psi_A(x)$ is an analytical function, its second derivative can be ignored (in the short time regime, all the non-singular terms have a negligible effects on the transition), and therefore, the equivalent singular wavefunction $\psi_S(x)$ needs only to maintain

$$V(x)\psi_A(x=0) = -\frac{\partial^2\psi_S(x)}{\partial x^2} \tag{6}$$

That is, any singularity in the potential $V(x)$ is equivalent to a corresponding singularity in the wavefunction $\psi_S(x)$; but, of course, the latter problem was practically solved.

The short time dynamics of the initial smooth $\psi_A(x)$ in the presence of the (singular) potential barrier will be exactly the