The Attractive Nonlinear Delta-Function Potential

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Abstract

We solve the continuous one-dimensional Schrödinger equation for the case of an inverted nonlinear delta–function potential located at the origin, obtaining the bound state in closed form as a function of the nonlinear exponent. The bound state probability profile decays exponentially away from the origin, with a profile width that increases monotonically with the nonlinear exponent, becoming an almost completely extended state when this approaches two. At an exponent value of two, the bound state suffers a discontinuous change to a delta–like profile. Further increase of the exponent increases again the width of the probability profile, although the bound state is proven to be stable only for exponents below two. The transmission of plane waves across the nonlinear delta potential increases monotonically with the nonlinearity exponent and is insensitive to the sign of its opacity.
The delta-function potential $\delta(x - x_0)$ has become a familiar sight in the landscape of most elementary courses on quantum mechanics, where it serves to illustrate the basic techniques in simple form. As a physical model, it has been used to represent a localized potential whose energy scale is greater than any other in the problem at hand and whose spatial extension is smaller than other relevant length scales of the problem. Arrays of delta-function potentials have been used to illustrate Bloch’s theorem in solid state physics and also in optics, where in the scalar approximation, wave propagation in a periodic medium resembles the dynamics of an electron in a crystal lattice. It is well known that the single “inverted” delta-function potential $-\Omega \delta(x - x_0)$ possesses one exponentially localized bound state for all values of the opacity parameter $\Omega$. Its existence and stability has been tested against the effects of different boundary conditions$^1$ and symmetry-breaking perturbations$^2$. In addition, the inverted delta potential has been used as a semi-permeable barrier to examine resonance phenomena in scattering theory$^3$, among others. Other interesting applications of the delta-function potential concept are found in Ref.4.

In this work we examine the problem of finding the bound state and the transmission coefficient of plane waves across an inverted non-linear delta–function potential, described by the so-called Nonlinear Schrödinger (NLS) equation:

$$\frac{\hbar^2}{2m} \phi''(x) - \frac{\hbar^2}{2m} \Omega \delta(x) |\phi(x)|^\alpha \phi(x) = E \phi(x),$$

where $\Omega > 0$ is the opacity coefficient and $\alpha$ is the nonlinearity exponent.
For $\alpha = 0$ we recover the familiar problem of the linear “inverted” delta-potential which possesses an exponentially decaying bound state profile for any opacity strength: $\phi(x) = \sqrt{\Omega/2} \exp(-\Omega/2 \cdot |x|)$. The rate of decay in space is determined by the localization length $2/\Omega$ which increases (decreases) as the opacity decreases (increases).

It might seem odd at first to see a nonlinear-looking Schrödinger equation like (1), since we know that quantum mechanics is linear. Therefore, all physical systems should be described by coupled sets of linear equations. However we oftentimes can only concentrate on a few “relevant” degrees of freedom, making suitable approximations to deal with the rest. At times, the price to pay for this reduction is the appearance of nonlinear evolution equations for the variables of interest, such as Eq. (1).

For instance, in atomic physics, a well-known approximation when dealing with multi-electron atoms is the self-consistent field approximation (Hartree-Fock). In this case each electron is described by a single-particle wave function that solves a Schrödinger-like equation. The potential appearing in this equation is that generated by the average motion of all the other electrons, and so depends on their single-particle wave functions. This results in a set of nonlinear eigenvalue equations\textsuperscript{5}. A more recent application of the mean-field ideas to a weakly interacting Bose condensate can be found in Ref.[6].

For $\alpha = 2$, Eq.(1) could model the problem of an electron propagating in a one-dimensional linear medium which contains a vibrational “impurity” at the origin that can couple strongly to the electron. In the approximation, where one considers the vibrations completely “enslaved” to the electron, one
obtains Eq.(1) as the effective equation for the electron.

A closely related equation, given by the discrete version of (1) is known as the discrete nonlinear Schrödinger (DNLS) equation. It was introduced in its time-independent form, in the late fifties by Holstein in his studies of the polaron problem in condensed matter physics. The DNLS equation was derived in a fully time-dependent form by Davydov in his studies of energy transfer in proteins and other biological materials. In the continuum limit the time-dependent DNLS equation reduces to the time-dependent NLS equation, which supports soliton solutions. Therefore, a soliton–based energy transport appears as an attractive candidate mechanism for energy transport in biomolecules. A recent review of the status of Davydov’s proposal can be found in Ref.[9]. The time-dependent DNLS equation can also be viewed as the evolution equation for a Hamiltonian system of classical anharmonic oscillators.

An important application of the continuous model (1) is that of a wave propagating in a one-dimensional linear medium which contains a narrow strip of nonlinear (general Kerr-type) material. This nonlinear strip is assumed to be much smaller than the typical wavelength. In fact, periodic and quasiperiodic arrays of nonlinear strips have been considered by a straightforward generalization of Eq.(1) in order to model wave propagation in some nonlinear superlattices.

Bound State ($E = E^{(b)} < 0$): Our system consists of a single, infinitely localized potential well in a continuous infinite line and therefore, lacks any natural length scale. If the delta potential were confined between two infinite
walls, the distance between the walls would provide a length scale. If, instead of a continuous line, the potential were defined on a discrete lattice, its lattice constant would define a natural length scale. Also, if instead of one delta potential, we had at least two of them, their mutual distance would constitute a natural length scale for the system.

In our case we have none of these. Thus, $\Omega$ serves only to define the unit of distance (as it does in the linear case). It is possible to get rid of $\Omega$ formally as follows: From Eq. (1) we see that $\Omega$ must have units of $[\text{distance}]^{(\alpha/2)-1}$, which suggests the definition of a dimensionless distance $u$ as $u = x/L$, with $L \equiv \Omega^{2/(\alpha-2)}$. In terms of $u$ and $\phi(u) \equiv (1/\sqrt{L}) \phi(x)$, Eq. (1) can be recast in a dimensionless form:

$$
\phi''(u) - k^2 \phi(u) = -\delta(u) |\phi(u)|^\alpha \phi(u),
$$

with $k^2 = -2mL^2E^{(b)}/\hbar^2$ and $\phi''(u) = (d^2/du^2)\phi(u)$. The opacity $\Omega$ has now disappeared from view since it only determines the unit of distance. We try:

$$
\phi(u) = \begin{cases} 
A \exp(k \ u) & u < 0 \\
B \exp(-k \ u) & u > 0 
\end{cases}
$$

Using the continuity of $\phi(u)$ and the discontinuity of $\phi'(u)$ at $u = 0$, one obtains $A = B$ and $k = (1/2) |A|^{\alpha}$. Finally, use of the normalization condition $1 = \int_{-\infty}^{\infty} |\phi(u)|^2 \, du$, leads to

$$
\phi(u) = \left(\frac{1}{2}\right)^{1/(2-\alpha)} \exp \left[-\left(\frac{1}{2}\right)^{2/(2-\alpha)} |u|\right]
$$

with a dimensionless bound state energy

$$
E^{(b)} = -\left(\frac{1}{2}\right)^{4/(2-\alpha)}.
$$
As in the linear ($\alpha = 0$) case, the bound state profile is exponentially decreasing away from the delta potential with localization length $2^{2/(2-\alpha)}$. As $\alpha$ increases from zero, the probability profile widens and the bound state energy decreases in magnitude. At $\alpha = 2^-$, the state is completely extended all over the real axis and the bound state energy is vanishingly small. At $\alpha = 2^+$, the bound state becomes infinitely localized, with a delta–like probability profile and with an infinite bound state energy. Further increase in the nonlinear exponent leads to a widening of the probability profile and to a corresponding reduction in the magnitude of the bound state energy.

Figure 1 shows the amplitude, or the inverse square probability profile width, of the bound state as a function of the nonlinearity exponent. However, at this point, an important observation is in order. The total energy of the system does not coincide with the bound state energy. In order to see this, we must consider the full time-dependent nonlinear Schrödinger equation that gives rise to Eq. (2). By using $\tau \equiv t/T$ as a dimensionless time variable, with $T \equiv (\hbar/2mL^2)^{-1}$, we have

$$i \frac{d}{d\tau} \psi(u, \tau) = -\frac{d^2}{d\tau^2} \psi(u, \tau) - \delta(u) |\psi(u, \tau)|^\alpha \psi(u, \tau). \quad (6)$$

In other words, we have $i(d/d\tau) \psi(u, \tau) = H \psi(u, \tau)$, where the Hamiltonian operator can be decomposed as $H = H_0 + O_{NL}$, where $H_0 = p^2$, with $p = i \frac{d}{du}$ and $O_{NL} = -\delta(u) |\psi(u, \tau)|^\alpha$ as the nonlinear part. We see that $H$ depends on time explicitly, through the time dependence of $O_{NL}$:

$$\frac{\partial H}{\partial \tau} = \frac{\partial O_{NL}}{\partial \tau}. \quad (7)$$
This implies that $\langle H \rangle$ is no longer a constant of the motion:

$$\frac{d\langle H \rangle}{d\tau} = i\langle [H, H] \rangle + \left\langle \frac{\partial H}{\partial \tau} \right\rangle = \left\langle \frac{\partial H}{\partial \tau} \right\rangle \neq 0. \quad (8)$$

For the nonlinear part, we have

$$\frac{d\langle O_{NL} \rangle}{d\tau} = i\langle [H, O_{NL}] \rangle + \left\langle \frac{\partial O_{NL}}{\partial \tau} \right\rangle. \quad (9)$$

But,

$$\left\langle \frac{\partial O_{NL}}{\partial \tau} \right\rangle = \int du |\psi(u, \tau)|^2 (\partial O_{NL}/\partial \tau). \quad (10)$$

By expressing $O_{NL}$ in terms of $\psi(u, \tau)$ and using Eq. (6), we can recast (10) as

$$\left\langle \frac{\partial O_{NL}}{\partial t} \right\rangle = \frac{i\alpha}{2} \langle [H, O_{NL}] \rangle, \quad (11)$$

which means

$$\frac{d\langle O_{NL} \rangle}{d\tau} = i \left( 1 + \frac{\alpha}{2} \right) \langle [H, O_{NL}] \rangle. \quad (12)$$

By comparing Eqs. (11) and (12), we conclude

$$\left\langle \frac{\partial O_{NL}}{\partial \tau} \right\rangle = \left( \frac{\alpha}{\alpha + 2} \right) \frac{d}{d\tau} \langle O_{NL} \rangle. \quad (13)$$

Finally, by inserting this back into Eq. (7), Eq. (8) becomes:

$$\frac{d}{d\tau} \langle H \rangle = \left( \frac{\alpha}{\alpha + 2} \right) \frac{d}{d\tau} \langle O_{NL} \rangle, \quad (14)$$

which implies

$$\frac{d}{d\tau} \left\langle H - \left( \frac{\alpha}{\alpha + 2} \right) O_{NL} \right\rangle = 0. \quad (15)$$

Therefore, the true energy operator for our system is $H_t \equiv H - (\alpha/\alpha+2) O_{NL}$.

For a stationary-state, $\psi(u, \tau) = \phi(u) \exp(-iE^{(b)}t/\hbar)$, the total dimensionless
energy is then
\[ E_t = E^{(b)} - \left( \frac{\alpha}{\alpha + 2} \right) (-\lvert \phi(0) \rvert^{\alpha+2}) = - \left( \frac{1}{2} \right)^{4/(2-\alpha)} \left( \frac{2 - \alpha}{2 + \alpha} \right). \] (16)

Thus, for \( \alpha < 2 \) the total energy is negative and the eigenstate is a stable localized state. On the contrary, when \( \alpha > 2 \), the total energy is positive and the eigenstate is localized but possibly unstable, which means that any weak ‘perturbation’ could make it disappear into the continuum. This explains the ‘stable’ and ‘unstable’ labelling in Fig. 1. Only for \( \alpha = 0 \), i.e., the linear case, both the total energy and the energy eigenvalue coincide. Figure 2 shows some probability profiles for several different values of the nonlinear exponent that give rise to true (stable) bound states. This distinction between the eigenenergy and the total energy must always be kept in mind when dealing with effectively nonlinear systems.

**Transmission of plane waves** \((E > 0)\): We now cast Eq.(1) as
\[ \psi''(x) + k^2 \psi(x) = -\Omega \delta(x) \lvert \psi(x) \rvert^\alpha \psi(x) \] (17)

where \( k^2 = 2mE/\hbar^2 \) is the electron wavevector. Unlike the bound state problem, we now have \( 1/k \) as a natural length scale and can therefore consider \( \Omega \) as a *bona fide* opacity coefficient. The problem looks similar to the usual single delta-barrier problem, with the exception of the nonlinear term \( \lvert \psi \rvert^\alpha \) that modulates the strength of the barrier opacity, depending on how much electronic probability is sitting on the barrier. We will examine the dependence of the transmission coefficient on \( \Omega \) and \( \alpha \).
Since we are interested in plane wave transmission, we set
\[
\psi(x) = \begin{cases} 
R_0 \exp(ikx) + R \exp(-ikx) & x < 0 \\
T \exp(ikx) & x > 0
\end{cases}
\] (18)

From the continuity of \(\psi(x)\) and discontinuity of \(\psi'(x)\) at \(x = 0\), we obtain
\[
T = R_0 + R
\] (19)
\[
iki T = i k (R_0 - R) - \Omega \left| T \right|^\alpha T.
\] (20)

From here, one obtains \(T = 2R_0/(2 - (i\Omega/k) \left| T \right|^\alpha)\). Defining the transmission coefficient as \(t \equiv \left| T \right|^2/\left| R_0 \right|^2\), we obtain the following equation for the transmission coefficient:
\[
t = \frac{4}{4 + (\Omega^*/k)^2 t^\alpha}
\] (21)

where \(\Omega^* \equiv \Omega|R_0|^\alpha\) is the “effective” opacity. We note that (21) is invariant under a sign change in \(\Omega\). In other words, both the “upright” and the “inverted” delta potentials possess identical transmissivities.

For arbitrary \(\alpha\), Eq. (21) is a nonlinear equation for \(t\) and must be solved numerically. There are, however, four exactly solvable cases, three of which can be described shortly:

1. \(\alpha = 0\) (linear case): From (21) we immediately obtain the well-known result
\[
t = \frac{1}{1 + (\Omega/k)^2}
\] (22)

2. \(\alpha = 1\): Now Eq. (21) can be recast as the quadratic equation \((\Omega^*/2k)^2 t^2 + t - 1 = 0\), with physical solution
\[
t = \frac{k}{\Omega^*} \left[-1 \pm \sqrt{1 + \frac{(\Omega^*/k)^2}{2}}\right]
\] (23)
3. $\alpha = 2$: Now we deal with a cubic equation for $t$: $(\Omega^*/2k)^2t^3 + t - 1 = 0$.

Its physical solution is

$$t = (2/9)^{1/3} (1/|\Omega^*|) \ A(k, \Omega^*) - (32/3)^{1/3} (k^2/|\Omega^*|) \ A(k, \Omega^*)^{-1/3}$$

(24)

where $A(k, \Omega^*) = 9k^2|\Omega^*| + \sqrt{3}(16k^6 + 27k^4\Omega^*)$

The case $\alpha = 3$ is exactly solvable in principle, but it leads to a cumbersome expression for $t$ that is not particularly illuminating.

If we recast the general equation for $t$ as $t \ (1 + (\Omega^*/2k)^2 \ t^\alpha) = 1$, a bit of simple analysis will convince the reader that the left hand side is always a monotonically increasing function of $t$ for $\alpha > 0$. Therefore, there is always only one solution in the interval $0 \leq t \leq 1$. Figure 3 shows the transmission coefficient $t$ as a function of $k/\Omega^*$ and several different nonlinearity exponents $\alpha$. Unlike the bound state calculation, there is no restriction here on the magnitude of the nonlinear exponent $\alpha$. For all wavevectors, the transmission increases with increasing $\alpha$ and does not display any special behavior at $\alpha = 2$. The increase of $t$ with $\alpha$ can be easily understood with the help of Eq.(21): For any $\alpha > 0$, $t^\alpha < 1$ since $t$ is less than unity. Thus, $\Omega^* \ t^\alpha < \Omega^*$ which means that the total “nonlinear” opacity is always smaller than the “linear” one, hence a higher transmission.

**Summary.** In this work we have calculated the bound state corresponding to a single “inverted” nonlinear delta-function potential, with opacity $\Omega$ and nonlinearity exponent $\alpha$. Following the usual methods of elementary quantum mechanics, we arrived at a closed form expression for the bound state characterized by an exponentially-decreasing probability profile, with
a localization length that decreases with increasing \( \alpha \). The most significant feature of this solution is the existence of a critical \( \alpha \) value, namely 2, beyond which the total energy (not the eigenenergy) of the bound state becomes positive, making the state unstable against a collapse into the continuum. The transmission of plane waves across the nonlinear delta potential is invariant under a sign change in opacity, and increases monotonically with an increasing nonlinearity exponent. The transmission is always higher than in the linear case, for a nonzero exponent.

Finally, it is important to remark that because of the nonlinear nature of Eqs. (1) and (3), it is no longer possible to superpose stationary states in order to find the time evolution of a given initial state. A stationary state solution of Eq. (3) is now only a particular solution whose relation to the solution of the time-dependent problem is unclear. Other features that arise in similar ‘nonlinear’ quantum mechanical problems include the fact that eigenstates are no longer guaranteed to be orthogonal to each other. Also, the number of eigenstates is no longer constant, but depends on nonlinearity. Thus, ‘nonlinear’ quantum mechanics is considerably more challenging than the linear one, although the reader should be aware that, as was mentioned at the beginning of this Note, nonlinearity in quantum mechanics is the consequence of some underlying assumption about the system.
ACKNOWLEDGMENTS

This work was supported in part by FONDECYT grants 1990960 (M.I.M), 2980033 (C.A.B) and 4990004 (C.A.B). The authors are grateful to J. Rössler for illuminating discussions.
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Captions List

**Fig.1**: Normalized bound state amplitude at the origin as a function of the nonlinearity exponent. The wavefunction changes discontinuously at $\alpha = 2$, becoming unstable for $\alpha > 2$.

**Fig.2**: Bound state probability profile for the “inverted” nonlinear delta-function potential, for several nonlinearity exponents $\alpha$ that give rise to a stable bound state.

**Fig.3**: Transmission coefficient of plane waves across the nonlinear delta-function potential versus wavevector, for several different nonlinearity exponent values. The transmission is the same for the “upright” and “inverted” delta potentials.
\[ \frac{\phi(0)}{(1/2)^{1/2}} \]

\( \alpha \)

STABLE

UNSTABLE

FIG. 1
FIG. 3

The graph represents the transmission as a function of $k/\Omega^*$ for different values of $\alpha$. The curves are labeled with $\alpha = 0, 1, 2, 3, 4$, showing how transmission changes with varying $\alpha$. The x-axis represents $k/\Omega^*$, and the y-axis represents transmission.