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Barrier transmission for the nonlinear Schrödinger equation: surprises of nonlinear transport

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Abstract

In this paper we report on a peculiar property of barrier transmission that systems governed by the *nonlinear* Schrödinger equation share with the linear one: for unit transmission the potential can be divided at an arbitrary point into two sub-potentials, a left and a right one, which have exactly the same transmission. This is a rare case of an exact property of a nonlinear wavefunction which will be of interest, e.g., for studies of coherent transport of Bose–Einstein condensates through mesoscopic waveguides.

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(Some figures in this article are in colour only in the electronic version)

Quantum mechanics is full of surprises, in some cases even in quite elementary situations, that are seemingly well known from textbooks. A recent example is the following remarkable observation for barrier penetration.

Let us consider the transmission of a one-dimensional wavefunction through a potential $V(x)$ with $V(x) \rightarrow 0$ for $x \rightarrow \pm\infty$. A well-known example is a rectangular potential well

$$V(x) = \begin{cases} -V_0, & |x| \leq a \\ 0, & |x| > a \end{cases} \quad (1)$$

($V_0 > 0$) with a transmission probability [1]

$$|T|^2(E) = \left\{ 1 + \frac{V_0^2}{4E(E + V_0)} \sin^2(2a\sqrt{2m(E + V_0)}/\hbar) \right\}^{-1} \quad (2)$$

(m is the mass of the particle and E is the energy). At certain ‘resonance’ energies E_{res} the potential is 100% transparent, for example at $E_n = -V_0 + (\hbar^2\pi^2/8ma^2)n^2 > 0$, $n = n_{\text{min}}, n_{\text{min}} + 1, \dots$, for the rectangular well (1). Such resonances have been studied for more general potentials, as for example symmetrical or asymmetrical double-barrier structures in connection with resonant-tunneling, where they are denoted as unit resonances (see, e.g., [2] and references therein).

Chabanov and Zakhariev [3] discovered that, at such a resonant energy, the potential scattering shows a surprising symmetry: dividing $V(x)$ into two distinct parts at some arbitrary point x' defining a 'left' and a 'right' potential

$$V_L(x) = \begin{cases} V(x), & x \leq x', \\ 0, & x > x', \end{cases} \quad V_R(x) = \begin{cases} 0, & x < x', \\ V(x), & x \geq x', \end{cases} \quad (3)$$

the transmission probabilities $|T_L|^2$ for V_L and $|T_R|^2$ for V_R are equal at the resonance energy,

$$|T_L|^2(E_{\text{res}}) = |T_R|^2(E_{\text{res}}), \quad (4)$$

despite the fact that the left and right potentials can be very different. This is shown easily using the transfer matrix \mathbf{M} connecting the amplitudes of the wavefunction on the left-hand side, $\psi(x) = A \exp(ikx) + B \exp(-ikx)$, with those on the right-hand side, $\psi(x) = C \exp(ikx) + D \exp(-ikx)$ (the limit $|x| \rightarrow \infty$ is understood for a potential not vanishing outside a finite range):

$$\begin{pmatrix} C \\ D \end{pmatrix} = \mathbf{M} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}, \quad (5)$$

where the unit determinant $\det \mathbf{M} = |\alpha|^2 - |\beta|^2 = 1$ guarantees that the reflection probability $|R|^2 = |\beta/\alpha|^2$ and the transmission probability $|T|^2 = 1/|\alpha|^2$ sum to unity (see, e.g., [1]). If the potential is cut at x' according to (3), the total transfer matrix can be expressed as a product of the transfer matrices \mathbf{M}_R and \mathbf{M}_L of the right and left potentials, respectively: $\mathbf{M} = \mathbf{M}_R \mathbf{M}_L$. For unit transmission we have $|\alpha| = 1$ and

$$\beta = \alpha_R \beta_L + \beta_R \alpha_L^* = 0 \quad (6)$$

which implies $\beta_R/\alpha_R = -\beta_L^*/\alpha_L$ and hence equal reflection probabilities of V_R and V_L . This property, which can also be extended to more general situations, offers an intuitive approach to the design of potentials with desired transmission properties (see [3] and references therein for more details).

In this paper we report an even more puzzling fact, namely that these properties remain valid for the nonlinear Schrödinger equation (NLSE)

$$\frac{\hbar^2}{2m} \psi'' + (\mu - V)\psi - g|\psi|^2\psi = 0. \quad (7)$$

The nonlinearity destroys the superposition principle in linear quantum mechanics and we therefore cannot base our proof on matrix techniques as above. The NLSE (7), also known as Gross–Pitaevskii equation, attracted much interest in recent years because it describes the dynamics of Bose–Einstein condensates in a mean-field approximation at low temperature (see, e.g., [4]). Note that the chemical potential μ takes over the role of the energy E . We furthermore note that also the nonlinearity g may be x dependent.

Transport properties of cold atomic gases in designed mesoscopic waveguides are of recent interest [5]. Here in particular barrier transmission of the nonlinear waves has been studied in a number of papers [5–8] that assume an experimental setup in which matter waves from a large reservoir of condensed atoms at chemical potential μ are injected into a one-dimensional waveguide in which the condensate can propagate. In these articles it was shown that the results obtained from the stationary NLSE (7) are in excellent agreement with numerical solutions of the time-dependent NLSE

$$i\hbar \dot{\psi}(x, t) = -\frac{\hbar^2}{2m} \psi''(x, t) + V(x)\psi(x, t) + g|\psi(x, t)|^2\psi(x, t) + f_0 \exp(-i\mu t/\hbar)\delta(x - x_0), \quad (8)$$

where the source term $f_0 \exp(-i\mu t/\hbar)\delta(x - x_0)$ located at $x = x_0$ emits monochromatic matter waves at chemical potential μ and thus simulates the coupling to a reservoir. The barrier potential $V(x)$ is assumed to be zero for $x \leq x_0$. As discussed in these articles, the definition of a transmission probability is not unambiguous, because of the implicit dependence on the scattering wavefunction $|\psi(x)|^2$. Different prescriptions assuming either a fixed source strength f_0 or a fixed incoming current can be formulated which differ in a strongly nonlinear situation. No ambiguity appears, of course, if the nonlinearity vanishes in the region far away from the scattering potential. Note that for unit transmission the differences between fixed output or input conditions as well as the definition ambiguities disappear. See [5, 8] for more details.

A fixed output boundary condition

$$\psi(x) \rightarrow C \exp(ikx), \quad \psi'(x) \rightarrow ikC \exp(ikx) \quad \text{for } x \rightarrow +\infty \quad (9)$$

with $k = \sqrt{2m(\mu - g|C|^2)}/\hbar$ determines the wavefunction $\psi(x)$ and its derivative $\psi'(x)$ in the region $-\infty \leq x \leq \infty$ uniquely [9]. This provides a recipe to define an effective incoming amplitude A in the upstream region and a transmission coefficient

$$|T|^2 = (k/k_A)|C/A|^2 \quad \text{with } k_A = \sqrt{2m(\mu - g|A|^2)}/\hbar. \quad (10)$$

For the fixed output problem, the transmission coefficient is a unique function of the chemical potential μ . If the problem is formulated as a fixed input problem, one observes a bending over of the transmission spectra and an interaction-induced bistability for strong nonlinearity where the transmission coefficient is no longer a unique function of μ . In addition, it was found that the points of unit transmission, the resonances μ_{res} , survive in the nonlinear case $g \neq 0$, of course shifted to different positions depending on g . In the following examples, we will use transmission coefficients derived from the fixed output condition (9).

If the potential $V(x)$ is 100% transparent at the chemical potential $\mu = \mu_{\text{res}}$, the solution in the far upstream region is given by

$$\psi(x) \rightarrow C \exp(ikx + i\varphi), \quad \psi'(x) \rightarrow ikC \exp(ikx + i\varphi) \quad \text{for } x \rightarrow -\infty, \quad (11)$$

where φ is a real-valued phase.

Now we define a second fixed output problem given by the NLSE

$$\frac{\hbar^2}{2m} \chi'' + (\mu - V)\chi - g|\chi|^2\chi = 0 \quad (12)$$

with the initial conditions

$$\chi(x) \rightarrow C^* \exp(-ikx - i\varphi), \quad \chi'(x) \rightarrow -ikC^* \exp(-ikx - i\varphi) \quad (13)$$

for $x \rightarrow -\infty$, which corresponds to scattering through $V(x)$ from the opposite side of the well. Noting that, for real values of μ , the complex conjugate of a solution also solves the NLSE, we find immediately that the solution of (12) and (13) is given by

$$\chi(x) = \psi^*(x), \quad \chi'(x) = \psi'^*(x), \quad (14)$$

and in particular

$$\chi(x) = C^* \exp(-ikx), \quad \chi'(x) = -ikC^* \exp(-ikx) \quad \text{for } x \rightarrow +\infty. \quad (15)$$

This means that the barrier potential $V(x)$ is also transparent for waves with chemical potential μ coming in from the opposite side of the barrier even if the potential is asymmetrical. Note that this is not satisfied automatically, because the equality of the left-to-right and right-to-left transmission probabilities valid in the linear case is not guaranteed for the NLSE, at least to the knowledge of the authors.

Now we divide the barrier potential $V(x)$ as given in equation (3) and obtain two new fixed output problems: the first one is determined by the NLSE

$$\frac{\hbar^2}{2m} \psi_R'' + (\mu - V_R) \psi_R - g |\psi_R|^2 \psi_R = 0 \quad (16)$$

with the initial conditions

$$\psi_R(x) \rightarrow C \exp(ikx), \quad \psi_R'(x) \rightarrow ikC \exp(ikx) \quad \text{for } x \rightarrow +\infty, \quad (17)$$

which corresponds to tunneling through the potential $V_R(x)$ from the left-hand side to the right-hand side of the barrier. The second one is determined by the NLSE

$$\frac{\hbar^2}{2m} \chi_L'' + (\mu - V_L) \chi_L - g |\chi_L|^2 \chi_L = 0, \quad (18)$$

with the initial conditions

$$\chi_L(x) \rightarrow C^* \exp(-ikx - i\varphi), \quad \chi_L' \rightarrow -ikC^* \exp(-ikx - i\varphi) \quad (19)$$

for $x \rightarrow -\infty$, which corresponds to tunneling through the potential $V_L(x)$ from the right-hand side to the left-hand side of the barrier.

From equation (14) we obtain at the cutting position x'

$$\chi_L(x') = \psi_R^*(x'), \quad \chi_L'(x') = \psi_R'^*(x'). \quad (20)$$

Since the wavefunctions in the respective potential-free regions are uniquely determined by the values of the wavefunction and its derivative at x' it follows together with the initial conditions (17) and (19) that the asymptotic wavefunction $\chi_L(x)$ for $x \rightarrow \pm\infty$ is equal to the asymptotic wavefunction $\psi_R^*(x)$ for $x \rightarrow \mp\infty$ up to an irrelevant phase factor $\exp(i\varphi)$. Thus the respective transmission coefficients coincide no matter which particular definition of the transmission coefficient is used.

For illustrative purposes we explicitly demonstrate in the following the equality of the two transmission coefficients for the case that a fixed source strength f_0 is assumed in equation (8). In section II.A of [8], it was shown that the source strength is connected with the effective incoming amplitude A_R via $f_0 = i \frac{\hbar^2}{m} k_R A_R$ with $k_R = \sqrt{2m(\mu - g|A_R|^2)\hbar}$. By considering the stationary solutions of equation (8) it was further shown that A_R is determined by the wavefunction and its derivative at the position x_0 of the source. Choosing $x_0 = x'$ we obtain from equation (12) in [8]

$$2ik_R A_R = \psi_R'(x') + ik' \psi_R(x') \quad (21)$$

with $k' = \sqrt{2m(\mu - g|\psi_R(x')|^2)\hbar} = \sqrt{2m(\mu - g|\chi_L(x')|^2)\hbar}$. Since $\chi_L(x)$ corresponds to scattering from the opposite direction the respective equation for the effective incoming amplitude A_L differs by a sign. With the definition $k_L = \sqrt{2m(\mu - g|A_L|^2)\hbar}$ we thus arrive at

$$2ik_L A_L = \chi_L'(x') - ik' \chi_L(x') = (\psi_R'(x') + ik' \psi_R(x'))^* = (2ik_R A_R)^* \quad (22)$$

using (20) and (21). Consequently, we obtain $|A_L|^2 = |A_R|^2$ and $k_L = k_R$ so that the respective transmission coefficients

$$|T_L|^2 = \frac{k|C|^2}{k_L|A_L|^2} = \frac{k|C|^2}{k_R|A_R|^2} = |T_R|^2 \quad (23)$$

coincide. More precisely, the left-to-right transmission of V_L is equal to the right-to-left transmission of V_R (compare the remark above).

As an illustration, we present results based on a numerical solution of the NLSE for two cases. Figure 1 shows the transmission probability for a rectangular well (1) with

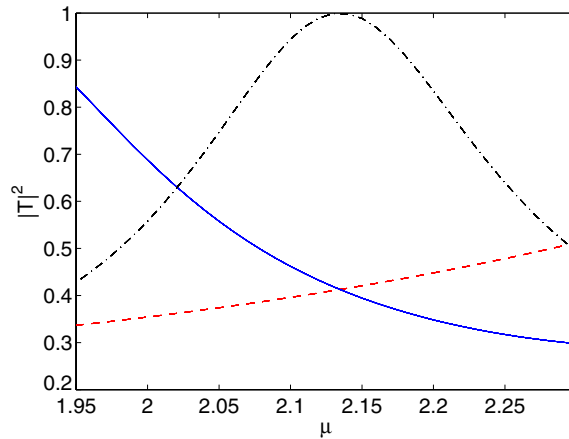


Figure 1. Transmission coefficient (---) of the NLSE for the rectangular potential well (1) (parameters $m = \hbar = 1$, depth $V_0 = 50$, width $2a = 40$ and attractive nonlinearity $g = -1$). Also shown are the transmission probabilities for the left (width 10, ---) and right potential (width 30, -) obtained from dividing $V(x)$ into two parts. These two probabilities are equal at the resonance at μ_{res} where the potential $V(x)$ is transparent.

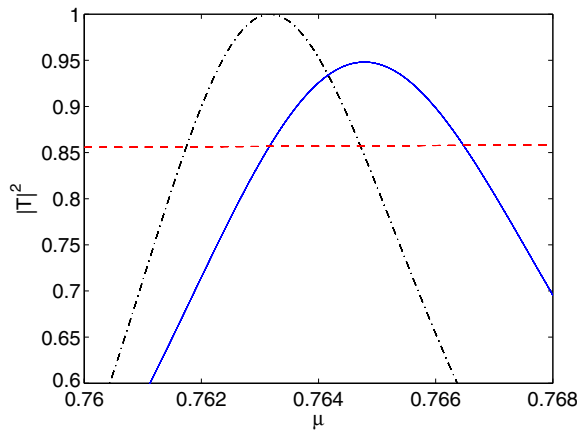


Figure 2. Same as figure 1, however for the double-barrier potential (24).

$m = \hbar = 1$, $V_0 = 50$, $a = 20$ and an attractive nonlinearity $g = -1$ acting along the whole x -axis. The outgoing boundary conditions are chosen as $C = 1$. We observe unit transmission, $|T|^2 = 1$, at the resonance $\mu_{\text{res}} \approx 2.135$.

We now divide the rectangular well with width $2a = 40$ at the value $x' = -10$ into two separate parts and calculate the transmission coefficient of each of these rectangular wells V_L (width 10) and V_R (width 30) separately. Their transmission curves displayed in figure 1 cross at the chemical potential μ_{res} , exactly as predicted.

As a second example we choose the double-Gaussian barrier

$$V(x) = V_0[\exp(-(x + b)^2/\alpha^2) + \exp(-(x - b)^2/\alpha^2)] \tag{24}$$

with parameters $V_0 = 1$, $b = 7.35$, $\alpha = b/5$ and a nonlinearity of $g = 0.005$ studied in [6, 8], where the apparently small value of g nevertheless causes a strong deviation of the nonlinear

resonance curve from the linear one. In figure 2 we observe full transparency at $\mu \approx 0.7632$, i.e. below the potential maxima. In addition the figure shows the transmission curves for the left and right potentials, where the potential is divided by $x = -8.0$. Again the left and right transmission coefficients are equal at the point of transparency.

In conclusion, we have shown that the interesting property of linear quantum barrier penetration at unit transmission, the equality of transmission through the arbitrarily divided sub-potentials, can be carried over to the nonlinear case which is much less understood. In addition of being of interest in its own right, this remarkable fact may provide an intuitive way to treat transport in nonlinear quantum systems, as for example the Bose–Einstein condensates in the mean-field approximation.

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