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1994 J. Phys. A: Math. Gen. 27 L439

(http://iopscience.iop.org/0305-4470/27/12/008)

J. Phys. A: Math. Gen. 27 (1994) L439–L445. Printed in the UK

LETTER TO THE EDITOR

Perfect absorbers for stationary and wavepacket scattering

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Received 7 March 1994

Abstract. Complex potentials that absorb the incoming wave in a finite distance without reflection or transmission are found by a simple inversion technique, both for stationary and wavepacket scattering in one dimension.

Collision processes in which annihilation or absorption of particles occur are often described by non-Hermitian potentials with an imaginary part. The best known complex-potential model is the optical model used in nuclear, atomic and molecular physics [1–3]. In this model a Schrödinger equation with an effective complex Hamiltonian describes the collision only in the channel(s) of interest. The effect of the complementary channels, which typically describe inelastic or reactive events, can, in principle, be accounted for exactly with the complex potential. Even though explicit formulae exist to obtain the exact effective Hamiltonian from the full interaction, the model is frequently used phenomenologically. This means that the complex potential is simply built to satisfy the physical requirement of fitting the experimental cross sections for the restricted processes of interest, especially when the number of open channels or complexity of the processes involved, in addition to the elastic or selected subspace of interest, is too large.

The experimental detection of particles by destructive procedures, for example, by means of the ionization of neutral species arriving at a detector in a crossed molecular-beam experiment, involves, in general, a complicated chain of events in which the annihilation of the scattered particles at the detector is just the first step. When comparing experimentally measured outgoing fluxes with theoretical results, in general, little thought is given to the possible effect of the detailed processes taking place in the detector. Actually, the implicit and hardly ever stated assumption is that the detector acts as a perfect absorber without reflection, i.e. without interfering significantly with the arriving part of the wave, up to the position of the detector. A related subject is the possibility to define and characterize quantum mechanical arrival times to spatially localized detectors. Again, the existence of a perfect absorber would clearly be a requirement to ignore the details of the detector and use the unperturbed fluxes in a valid quantum mechanical definition of the time of arrival [4–8].

These are not the only subjects in which complex potentials are important. In recent years, wavepacket methods have found a formidable development thanks to new algorithms and faster computers [9]. However, one of the technical difficulties is that most of these methods confine the packet to a finite sized box in coordinate space, so that for some applications the spurious collision with the boundary interferes with the true physical effects. A way out has been the use of absorbing imaginary potentials [10–13]. In this context a perfect absorber would be of obvious practical interest.

0305-4470/94/120439+07$19.50

In summary, potentials that absorb all the incoming flux in a limited spatial domain are of importance, both for fundamental reasons (to justify and model the connection between experimental scattering data and the usual theoretical treatments that simply ignore any detector effects) and for practical purposes (in wavepacket scattering computations). In fact there is a somewhat widespread belief that the perfect absorber does not exist [14, 15], and that reflection and/or transmission are unavoidable. Many attempts to find it have only provided partial results and no potential having strictly zero transmission and reflection has been described up to now. In this letter we construct perfect absorbers for stationary and wavepacket scattering.

The discussion is limited to a particle of mass m moving in one spatial dimension y, and interacting with a complex potential $v(y)$, which is chosen to be 0 for negative coordinates, region I, and ∞ for $y > L$, so that the transmission is zero. It is now convenient to divide the stationary Schrödinger equation with energy eigenvalue ϵ by $s \equiv \hbar^2/(2mL^2)$. Thus, using the dimensionless quantities $x = y/L$, $E = \epsilon/s$ and $V = v/s$, the equation takes the form

$$-\psi'' + V\psi = E\psi \tag{1}$$

where the prime indicates the derivative with respect to x. In region I, a stationary flux of incident and reflected particles at fixed energy is described by

$$\psi_{\mathrm{I}}(x) = \exp(\mathrm{i}kx) + R(k)\exp(-\mathrm{i}kx) \qquad x < 0 \tag{2}$$

where $k = E^{1/2}$ is the dimensionless wavenumber. We look for the form of a complex potential in region II ($0 < x < 1$) that causes no reflection at $k = k_0$, i.e. $R(k_0) = 0$. The following boundary conditions are imposed on the stationary wavefunction for region II:

$$\psi_{\mathrm{II}}(1) = 0 \tag{3}$$

$$\psi_{\mathrm{II}}(0) = \psi_{\mathrm{I}}(0) \tag{4}$$

$$\psi'_{\mathrm{II}}(0) = \psi'_{\mathrm{I}}(0)\,. \tag{5}$$

The first one corresponds to the infinite potential boundary at $x = 1$, where the derivative is not fixed. The last two equations are the usual matching conditions for the function and its derivative between regions I and II. It could seem that there are too many conditions for a second-order differential equation whose general solution admits only two arbitrary constants. However, note that the potential has not yet been specified and remains undetermined. Precisely, our inversion procedure consists of solving for $V(x)$ in the stationary Schrödinger equation

$$V(x) = E + \psi''(x)/\psi(x) \qquad 0 < x < 1 \tag{6}$$

by assuming a functional form for ψ_{II} able to fit the three conditions (3)–(5). The simplest is the quadratic form $\psi_{\mathrm{II}} = a_2x^2 + a_1x + a_0$. By substituting in (3)–(5) and using (2), one obtains

$$a_2 = -(1 + \mathrm{i}k_0) \tag{7}$$

$$a_1 = \mathrm{i}k_0 \tag{8}$$

$$a_0 = 1\,. \tag{9}$$

This gives the following perfect absorber at $k = k_0$:

$$V(x) = \begin{cases} 0 & x < 0 \\ k_0^2 + 2(x-1)^{-1}\left(x + \dfrac{1}{1+\mathrm{i}k_0}\right)^{-1} & 0 < x < 1 \\ \infty & x > 1 \end{cases} \tag{10}$$

which, on the real axis, has only two singular points, one at each extreme of region II. The first one is a finite discontinuity and the second is associated with a simple pole and the infinite barrier.

The above potential does not guarantee the absence of reflection for plane waves in a neighbourhood of k_0, say at $k_1 = (E_1)^{1/2} = k_0 + \delta k$. In other words, the derivative of the reflection coefficient $\mathrm{d}R/\mathrm{d}k|_{k_0}$ is not necessarily zero†. In fact, for practical applications it is desirable to find potentials absorbing an entire wavepacket, and not just a stationary wave with fixed momentum. To this end we may impose that, in addition to $R(k_0)$, $\mathrm{d}R/\mathrm{d}k|_{k_0}$ and higher derivatives are zero. The higher the order of vanishing derivatives, the flatter $R(k)$ will be in the neighbourhood of k_0, and the wider the momentum spread of the fully absorbed packets will be. The construction method used for the stationary case will be generalized in successive orders of the increment δk corresponding to the vanishing of derivatives of increasing order.

For a given potential function, two solutions of the stationary Schrödinger equation (1) at energies E_0 and E_1 (with subscripts 0 and 1, respectively) obey

$$(E_0 - E_1)\psi_0\psi_1 = W'(\psi_0, \psi_1) \tag{11}$$

where $W(\psi_0, \psi_1) = \psi_0\psi_1' - \psi_1\psi_0'$ is their Wronskian. In region I this equation is satisfied by the incoming plane waves $\mathrm{e}^{\mathrm{i}k_0 x}$ and $\mathrm{e}^{\mathrm{i}k_1 x}$. The following discussion refers to region II, but the subindex II is dropped out. Expanding the solution ψ_1 as $\psi_0 + f^{(1)}(x)\delta k + f^{(2)}(x)\delta k^2 + \cdots$, equation (11) becomes

$$\begin{aligned}(-2k_0\,\delta k - \delta k^2)(\psi_0^2 + \psi_0 f^{(1)}\delta k + \psi_0 f^{(2)}\delta k^2 + \cdots) \\ = \psi_0(\psi_0'' + f^{(1)''}\delta k + f^{(2)''}\delta k^2 + \cdots) - \psi_0''(\psi_0 + f^{(1)}\delta k + f^{(2)}\delta k^2 + \cdots).\end{aligned} \tag{12}$$

Equating terms of the same order on both sides (the zeroth-order terms lead to a trivial identity) gives

$$W'(\psi_0, f^{(1)}) = -2k_0\psi_0^2 \tag{13}$$

$$W'(\psi_0, f^{(2)}) = -2k_0\psi_0 f^{(1)} - \psi_0^2 \tag{14}$$

$$\vdots$$

$$W'(\psi_0, f^{(n)}) = -2k_0\psi_0 f^{(n-1)} - \psi_0 f^{(n-2)}. \tag{15}$$

The boundary conditions for $f^{(n)}$ are fixed by expanding ψ_1 in (3)–(5) around k_0 and comparing terms of equal order, with the understanding that in region I there is only an incoming wave,

$$f^{(1)}(0) = 0 \tag{16}$$

$$f^{(1)'}(0) = \mathrm{i} \tag{17}$$

$$f^{(1)}(1) = 0 \tag{18}$$

$$f^{(n)}(0) = f^{(n)'}(0) = f^{(n)}(1) = 0 \qquad n > 1. \tag{19}$$

Moreover, ψ_0 has to be consistent with conditions (2)–(5) for E_0, with $R(k_0) = 0$. Since the general expressions of the function and of the derivative at $x = 0$ are $\psi_1 = 1 + R(k_1)$ and $\psi_1'(0) = \mathrm{i}k_1[1 - R(k_1)]$, see equation (2); the condition of having only incoming wave in I amounts to assuming that for each order the corresponding derivative of R vanishes, as can be seen by expanding R around k_0.

† The modulus of the condition $\mathrm{d}R/\mathrm{d}k|_{k_0} = 0$, is not equivalent to the condition $\mathrm{d}|R|/\mathrm{d}k|_{k_0} = 0$. In particular, the potential (10) satisfies the latter, but not the former.

Next the first order is described in detail. Now a second-order inhomogeneous linear differential equation for the unknown function $f^{(1)}$ has to be solved, equation (13). If we again assume a quadratic form for ψ_0 the potential is fixed, as in the stationary case, by the boundary conditions for E_0, but then there is an excess of conditions for $f^{(1)}$ that cannot be satisfied in general. It is thus necessary to increase the degree of the polynomial so as to leave one indeterminate parameter in ψ_0. By substituting the cubic form $\psi_0 = b_3x^3 + b_2x^2 + b_1x + b_0$ in (3)–(5) one obtains

$$b_2 = -(1 + ik_0 + b_3) \tag{20}$$

$$b_1 = ik_0 \tag{21}$$

$$b_0 = 1 \tag{22}$$

where b_3 is the free parameter. The three roots of the cubic equation $\psi_0 = 0$ are

$$r_1 = 1 \tag{23}$$

$$r_{2,3} = (2b_3)^{-1}\left[(1 + ik_0) \pm (1 - k_0^2 + 2ik_0 + 4b_3)^{1/2}\right]. \tag{24}$$

Irrespective of the value of b_3 it is impossible for the three roots to be equal to 1, therefore the singular point at $x = 1$ is always regular or non-essential.

Disregarding the vanishing condition of $f^{(1)}$ at 1, equation (18), a solution of equation (13) subject to the initial conditions (16) and (17) depends parametrically on b_3. It will be denoted as $f_0^{(1)}(x; b_3)$. The problem of finding a perfect absorber for k_0 and $k_0 + \delta k$, having a vanishing first derivative of the reflection coefficient with respect to k at k_0, reduces to finding roots of $f_0^{(1)}(1; b_3)$ as a function of b_3, i.e. values of the parameter that also satisfy the boundary condition (18). By expanding the solution $f_0^{(1)}(x; b_3)$ in a power series around $x = 0$ and substituting in (13), a recurrence relation for the expansion coefficients is found. The convergence of the series far from $x = 0$ is, however, too slow for actual computations. Also, a series solution exists around the singular point $x = 1$, with similar difficulties at small x. By fixing its value as 0 at $x = 1$, it depends on b_3 and on an extra parameter γ fixing its derivative at that point. We shall call this particular solution $f_1^{(1)}(x; b_3, \gamma)$. b_3 can be obtained by matching at some intermediate point x_0 the series around $x = 0$ and the one around $x = 1$, as well as their derivatives. This amounts to solving the two homogeneous equations $f_0^{(1)}(x_0; b_3) - f_1^{(1)}(x_0; b_3, \gamma) = 0$ and $f_0^{(1)'}(x_0; b_3) - f_1^{(1)'}(x_0; b_3, \gamma) = 0$ for the two unknowns b_3 and γ. A practical way to do so is the Levenberg–Marquardt algorithm†.

Another option is to separate the second-order differential equation (13) into real and imaginary parts. These are easily converted into four coupled first-order differential equations that can be solved numerically by standard subroutines to provide the function $f_0^{(1)}(1; b_3)$ with initial conditions determined by (16) and (17). The zeros of this function can be efficiently found using Muller's method. Once b_3 has been fixed the potential is finally obtained in an explicit form from (6), putting $E = E_0$ and $\psi = \psi_0$, with the rest of the parameters of the cubic given by (20)–(22). Figures 1 and 2 show the real and imaginary parts of the zeroth (stationary), and first-order potentials for $k_0 = 1$.

Higher orders are discussed next. The second order requires one to solve the two coupled second-order differential equations (13) and (14) for $f^{(1)}$ and $f^{(2)}$. If ψ_0 is chosen as a polynomial, a quartic form $\psi_0 = c_4x^4 + c_3x^3 + c_2x^2 + c_1x + c_0$ that leaves two (complex) parameters free, c_4 and c_3, is needed to satisfy all boundary conditions for $f^{(1)}$ and $f^{(2)}$. As in the first-order case, it is convenient to separate (13) and (14) into real and imaginary parts and then convert the resulting four second-order equations into eight coupled first-order equations. The solutions $f^{(1)}(1; c_3, c_4)$ and $f^{(2)}(1; c_3, c_4)$ with the initial

† We have used IMSL's math library.

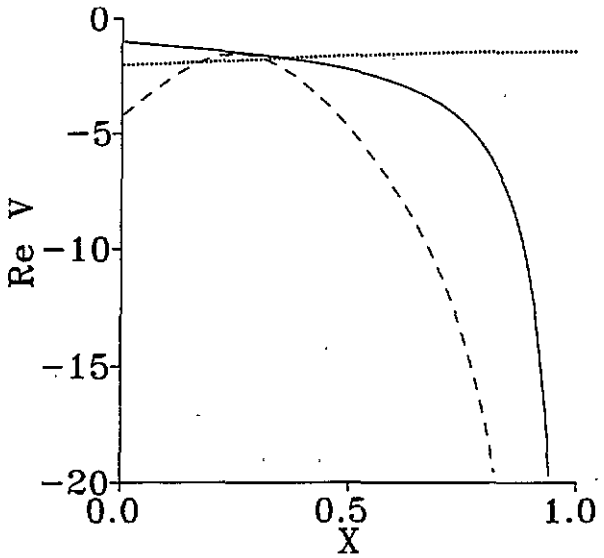

Figure 1. Real part of the complex potential $V(x)$ for $k_0 = 1$. Full curve: zeroth-order quadratic ψ_0; dotted curve: zeroth-order cubic ψ_0; broken curve: first-order cubic ψ_0, $b_3 = 1.6383 - i\,4.6607$.

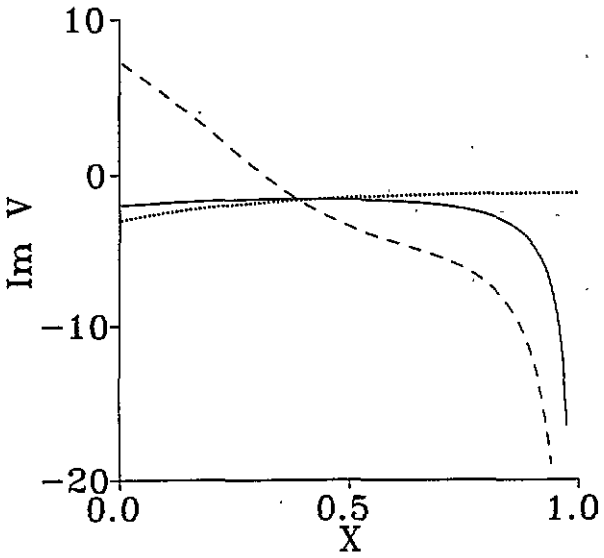

Figure 2. Imaginary part of the complex potential $V(x)$ for $k_0 = 1$. Same cases as figure 1.

conditions at $x = 0$ depend parametrically on c_3 and c_4. One is then left with the problem of finding zeros of the functions $f^{(1)}(1; c_3, c_4)$ and $f^{(2)}(1; c_3, c_4)$, which is equivalent to solving a homogeneous system of nonlinear equations for the unknowns c_3 and c_4. Again,

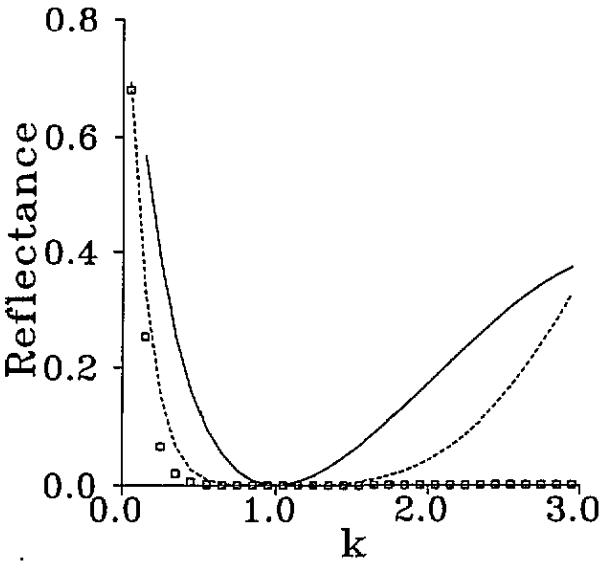

Figure 3. Reflectance, $|R|^2$, versus k for absorbing potentials with $k_0 = 1$. Full curve: zeroth-order potential, quadratic ψ_0; broken curve: first-order potential, cubic ψ_0, $b_3 = 1.6383 - i4.6607$; squares: second-order potential, quartic ψ_0, $c_3 = 0.1894 - i30.3240$, $c_4 = 4.283\,72 + i22.445\,31$. The reflectance of the second-order potential is less than 0.01 until $k \approx 5.4$.

an efficient method is the Levenberg–Marquardt algorithm. The third and higher orders can be handled similarly. Figure 3 shows the progressive flattening of the reflectance $|R(k)|^2$ for zeroth-, first- and second-order potentials. $R(k)$ at $k \neq k_0$ is computed by adapting the variable-phase method for s waves to our one-dimensional system [16].

In summary, perfect absorbers in a finite spatial range exist, and a method of construction has been described. Explicit functional forms have been obtained. The non-uniqueness of these potentials should be emphasized. Different functional forms can be proposed for ψ_0 to fit particular needs. As an example, in the stationary case the decay to $-\infty$ can be avoided by using a cubic form instead of a quadratic one, and imposing the extra condition $\psi_0''(1) = 0$, see figures 1 and 2. The polynomials chosen here appear as a simple and easily tractable choice. Also, for a given functional form of ψ_0 there can be more than one set of parameters that solve the coupled differential equations with the required boundary conditions, and therefore more than one potential. In forthcoming publications further analysis of these potentials will be carried out.

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