

# Chapter 15

## One-Dimensional Piecewise-Constant Potentials



After examining scattering by a potential step, we consider the finite potential well and the potential barrier. The physical phenomena we explore include discrete energy spectra and the tunnel effect. Finally, we show by example how to construct physically reasonable solutions by superposing (unphysical) partial solutions.

In a discussion of the stationary SEq, a major problem is that there are only very few realistic potentials for which closed solutions exist. To make analytical statements, one therefore almost always has to introduce approximations or simplifying assumptions; apart from that, one depends on numerical results.<sup>1</sup> This also applies to the one-dimensional case to which we restrict ourselves here. In this chapter, we simplify typical potentials by replacing them with ‘steps’,<sup>2</sup> i.e. by piecewise constant potentials; see Fig. 15.1.<sup>3</sup> As long as we do not assume that there are infinitely high potential walls at an arbitrary distance, we will also have to deal with continuous spectra.

Despite their schematic nature, the potentials discussed in this chapter are somewhat more realistic models of physical situations than the cases considered in Chap. 5, Vol. 1, i.e. the infinite potential well and free particle motion. We first consider a potential step, and then we will investigate in more detail bound and free states in some other potentials.

Using the example of the potential step, we discuss at the end of the chapter how to get physically reasonable solutions (also called *wave packets*) by the superposition of partial solutions (i.e. plane waves). We remind the reader that the superposition principle holds, due to the linearity of the SEq.

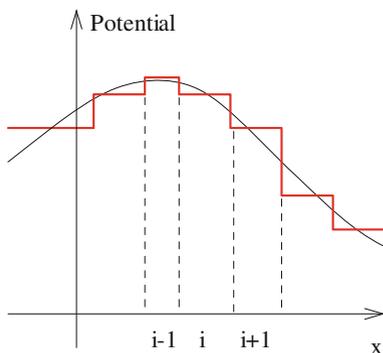
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<sup>1</sup>Books on quantum mechanics would be significantly thinner if one could solve the SEq for arbitrary potentials in closed form.

<sup>2</sup>We discuss approximation techniques in Chap. 19.

<sup>3</sup>We obtain exact solutions in this way. In principle, one can make the subdivision finer and finer and thus approximate the ‘true’ potential with arbitrary accuracy, but then the computational complexity increases disproportionately.

**Fig. 15.1** Approximation of a potential by a piecewise constant potential. In the region  $i$ , the potential is approximated by the constant value  $V_i$



Although one-dimensional piecewise constant potentials usually are addressed in undergraduate courses on atomic physics, we will discuss them in some detail again here for the sake of completeness.

## 15.1 General Remarks

We first discuss the solutions in each region of constant potential and then consider how to put together these partial solutions in the right manner.

In the region  $i$ , where the potential has the constant value  $V_i$ , the stationary SEq reads<sup>4</sup>

$$E\varphi_i(x) = -\frac{\hbar^2}{2m}\varphi_i''(x) + V_i\varphi_i(x). \quad (15.1)$$

It follows that

$$\varphi_i'' = \frac{2m}{\hbar^2}(V_i - E)\varphi_i, \quad (15.2)$$

which is the well-known second-order differential equation with constant coefficients that can be solved by an exponential *ansatz*. The prefactor of  $\varphi_i$  on the right-hand side is a constant for which a certain notation has become broadly established, namely  $\kappa$  and  $k$ :

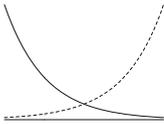
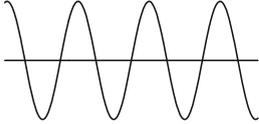
$$\begin{aligned} \kappa_i^2 &= \frac{2m}{\hbar^2}(V_i - E) \text{ for } V_i > E \\ k_i^2 &= -\frac{2m}{\hbar^2}(V_i - E) \text{ for } V_i < E, \end{aligned} \quad (15.3)$$

where  $\kappa_i, k_i > 0$  is assumed in general. Accordingly, we find two types of solutions:

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<sup>4</sup>The total energy  $E$  is the same everywhere, of course; the quantities which vary are the potential energy  $V_i$  and the kinetic energy  $E_{\text{kin}} = E - V_i$ .

**Table 15.1** Scheme of the two types of solutions

$E < V_i$	$E > V_i$
Classically forbidden region	Classically allowed region
$\varphi''(x) = \frac{2m}{\hbar^2} (V_i - E) \varphi(x) = \kappa^2 \varphi(x)$	$\varphi''(x) = -\frac{2m}{\hbar^2} (E - V_i) \varphi(x) = -k^2 \varphi(x)$
Exponential solution $e^{\pm\kappa x}$	Oscillatory solution $e^{\pm ikx}$
	

$$\begin{aligned} \varphi_i &= A_i e^{\kappa_i x} + B_i e^{-\kappa_i x} \quad \text{for } V_i > E \\ \varphi_i &= A_i e^{ik_i x} + B_i e^{-ik_i x} \quad \text{for } V_i < E \end{aligned} \tag{15.4}$$

i.e. an exponential or an oscillatory solution, depending on the sign of  $V_i - E$ .<sup>5</sup> The constants  $A$  and  $B$  are integration constants.

We have thus found a characteristic difference between quantum mechanics and classical mechanics. In classical mechanics, the total energy cannot be less than the potential energy, since this would imply a negative kinetic energy. The point at which is  $E = V$  is called the *classical turning point*. At this point, a classical particle must turn back, i.e. it is reflected. In quantum mechanics, there is a solution for the regions with  $V_i > E$ , the *classically forbidden regions*. This means that the quantum object penetrates into these regions in some sense. These solutions behave exponentially, while in the *classically allowed regions* (that is  $V_i < E$ ), they are oscillatory. The distinction between the two types of solutions is central to the present chapter. They are summarized in Table 15.1 and in Fig. 15.2.

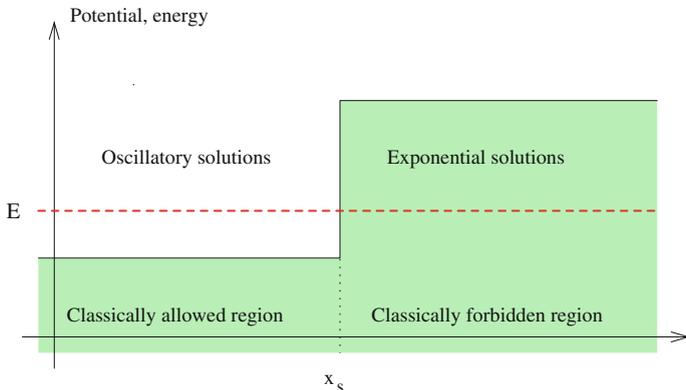
Hence, we can specify a solution for each region  $i$ . But how do we put together the partial solutions from each region, or in other words, how do we determine the constants of integration? Let us assume that the potential jumps at  $x_s$  (=point of discontinuity). Then we require that the different pieces of the wavefunction merge into each other ‘smoothly’. This requirement is motivated by the fact that we interpret  $\rho = \Psi^* \Psi$  as a probability density. In order for it to be physically reasonable, it has to be defined everywhere, e.g. it cannot have discontinuities. That is, the wavefunctions to the right and left of the discontinuity  $x_s$  of the potential,  $\varphi_{\text{left}}$  and  $\varphi_{\text{right}}$ , must be equal at  $x_s$  (continuity of the wavefunction):

$$\varphi_{\text{left}}(x_s) = \varphi_{\text{right}}(x_s). \tag{15.5}$$

Likewise, we require that the probability current density

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<sup>5</sup>It should again be noted that, from a physical point of view, exponential solutions  $\sim e^{\pm\kappa x}$  and oscillatory solutions  $\sim e^{\pm ikx}$  are worlds apart.



**Fig. 15.2** At the *left*: classically allowed region. At the *right*: classically forbidden region

$$j = \frac{\hbar}{2mi} (\varphi^* \varphi' - \varphi \varphi'^*) \quad (15.6)$$

and hence the derivative of the wavefunction be defined everywhere, which leads to:

$$\varphi'_{\text{left}}(x_s) = \varphi'_{\text{right}}(x_s). \quad (15.7)$$

Equations (15.5) and (15.7), together with the requirement on the behavior at infinity (or the boundary conditions), allow us to determine all the integration constants—apart from one which must necessarily stay undetermined because of the linearity of the SEQ. This one constant is at our disposition (we can choose it in such a way that e.g. the wavefunction is normalized).

A remark concerning infinitely high potentials: At the discontinuity of a finite to an infinite potential value, we can make a statement only about the wavefunction, not about its derivative. This means that we have only (15.5), i.e.,  $\varphi_{\text{left}}(x_s) = \varphi_{\text{right}}(x_s) = 0$ , while (15.7) does not apply here. More on this issue in Sect. 15.5.

In principle, we have thus solved the problem. However, the calculations are quite tedious even for only roughly ‘realistic’ potentials. Therefore, we first address the simplest example, namely the potential step.

## 15.2 Potential Steps

A quantum object, modelled by a plane wave, is incident from the right on a potential step. The potential is given by

$$V = \begin{cases} V_0 & \text{for } x < 0, \text{ region 2} \\ 0 & \text{for } x > 0, \text{ region 1.} \end{cases} \quad (15.8)$$

Accordingly, we have in region 1 the equation  $\varphi_1'' = -k^2\varphi_1$  with the solution

$$\varphi_1 = Ae^{ikx} + Be^{-ikx}; \quad k^2 = \frac{2mE}{\hbar^2} > 0; \quad A, B \in \mathbb{C}. \quad (15.9)$$

The term  $Be^{-ikx}$  represents the incoming wave and  $Ae^{ikx}$  the outgoing (scattered) wave.

We repeat the remark that the term ‘wave’ is actually wrong, because  $e^{-ikx}$  is a time-independent spatial oscillation, not a wave. Nevertheless, this term has become prevalent since one has the factor  $e^{-i\omega t}$  in mind and assumes  $k > 0$  and  $\omega > 0$ . Otherwise, expressions like ‘a plane wave, travelling to the left’ for  $e^{-ikx}$  would not make sense.

The solution in region 2 depends on whether  $E$  is less than or greater than  $V_0$ . Classically, one expects the following behavior: For  $E < V_0$ , the particle does not have enough energy to overcome the potential step, and is simply reflected. In the case  $E > V_0$ , however, the particle is not reflected, but propagates across the potential step (with reduced kinetic energy or velocity). Quantum mechanically, this is different. In the first case, the quantum object is able to enter the potential step (i.e. to enter a classically forbidden region). In the second case, the quantum object can be reflected, although it actually has enough kinetic energy to overcome the potential step. These two modes of behavior are purely quantum mechanical and quite different from classical mechanics. In Fig. 15.3, the situation is sketched.

We consider first the case  $E < V_0$  and then  $E > V_0$ .

### 15.2.1 Potential Step, $E < V_0$

In region 2 ( $x < 0$ ), we have  $\varphi_2'' = \frac{2m}{\hbar^2}(V_0 - E)\varphi_2 = \kappa^2\varphi_2$ , with the solution

$$\varphi_2 = Ce^{\kappa x} + De^{-\kappa x}; \quad \kappa^2 = \frac{2m}{\hbar^2}(V_0 - E) > 0; \quad C, D \in \mathbb{C}. \quad (15.10)$$

In this equation, we can determine one of the two coefficients by asking for physically reasonable behavior at infinity.<sup>6</sup> We see that in the limit  $x \rightarrow -\infty$ , the solutions are not bounded for  $D \neq 0$ . It follows that only for  $D = 0$  is the solution physically acceptable.

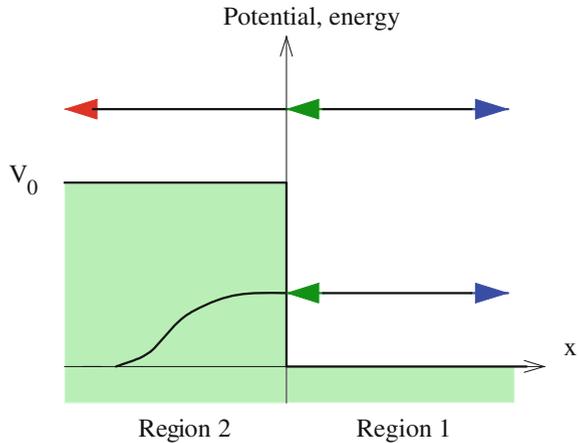
#### 15.2.1.1 Matching at the Discontinuity

The discontinuity of the potential lies at  $x = 0$ ; here we have  $\varphi_1 = \varphi_2$  and  $\varphi_1' = \varphi_2'$ . This leads to

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<sup>6</sup>Thus, concerning the validity of solutions, we have a criterion at hand which is not available for mathematics. This is a very nice plus for physics.

**Fig. 15.3** Situation for the potential step; above:  $E > V_0$ , below:  $E < V_0$ . The horizontal lines indicate an oscillation, the curved line an exponential decay. Incoming green, reflected blue, transmitted red



$$A + B = C; \quad ikA - ikB = \kappa C \quad (15.11)$$

These are two equations with three unknowns. We solve for  $A$  and  $C$  as a multiple of  $B$ , the amplitude of the incoming wave. We obtain:

$$A = B \frac{\kappa + ik}{ik - \kappa} \quad \text{and} \quad C = \frac{2ik}{ik - \kappa} B. \quad (15.12)$$

This leads to the result:

$$\begin{aligned} \varphi_1 &= B e^{-ikx} + B \frac{\kappa + ik}{ik - \kappa} e^{ikx} \quad \text{in region 1} \\ \varphi_2 &= \frac{2ik}{ik - \kappa} B e^{\kappa x} \quad \text{in region 2.} \end{aligned} \quad (15.13)$$

In region 2, the classically forbidden region, we have an exponentially decaying term. That means that there is ‘something’, where nothing should be according to the classical point of view. If one takes instead of the infinite potential step a potential barrier of finite width (which we will do below), this ‘something’ is released on the other side of the barrier—it has ‘tunneled’ through the barrier.

## 15.2.2 Potential Step, $E > V_0$

In region 2, we have the differential equation  $\varphi_2'' = -\frac{2m}{\hbar^2} (E - V_0) \varphi_2 = -k'^2 \varphi_2$ , with the solution:

$$\varphi_2 = A_2 e^{ik'x} + B_2 e^{-ik'x}; \quad k'^2 = \frac{2m}{\hbar^2} (E - V_0) > 0; \quad A_2, B_2 \in \mathbb{C}. \quad (15.14)$$

We see that this equation contains a wave travelling to the left ( $B_2e^{-ik'x}$ ) and another travelling to the right ( $A_2e^{ik'x}$ ). If we now let a quantum object be incident on the potential step from the right, we can exclude that a wave running from the left to the right exists in region 2, (i.e. coming from  $-\infty$ ). Therefore, we have  $A_2 = 0$  and the solution in region 2 reads:

$$\varphi_2 = B_2e^{-ik'x}. \quad (15.15)$$

This part of the wave is called the *transmitted* wave.

### 15.2.2.1 Matching at the Discontinuity

We have again three unknown variables, namely  $A$ ,  $B$  and  $B_2$ . The matching conditions for  $\varphi_1$  in (15.9) and  $\varphi_2$  in (15.15) at  $x = 0$  are  $\varphi_1 = \varphi_2$  and  $\varphi'_1 = \varphi'_2$ . It follows that

$$B_2 = A + B \quad \text{and} \quad -ik'B_2 = ikA - ikB. \quad (15.16)$$

The constants  $A$  and  $B_2$  are given by

$$A = B \frac{k - k'}{k + k'}; \quad B_2 = B \frac{2k}{k + k'} \quad (15.17)$$

and the solutions by:

$$\varphi_1 = Be^{-ikx} + B \frac{k - k'}{k + k'} e^{ikx}; \quad \varphi_2 = B \frac{2k}{k + k'} e^{-ik'x}. \quad (15.18)$$

### 15.2.2.2 Partial Waves: Transmission Coefficient and Reflection Coefficient

The facts can be summarized as follows: A wave coming from the right (corresponding to  $e^{-ikx}$ ) is incident on the potential step and is transmitted, i.e. continues to travel in that direction (with a different energy or wave number). In addition, we have a reflected wave—and that is something that absolutely does not exist in classical mechanics, comparable to a truck forced off the road by a mosquito flying against its windshield.<sup>7</sup> Accordingly, we can identify three partial waves:

$$\begin{aligned} \varphi_{\text{in}} &= Be^{-ikx} \\ \varphi_{\text{refl}} &= B \frac{k - k'}{k + k'} e^{ikx} \\ \varphi_{\text{trans}} &= B \frac{2k}{k + k'} e^{-ik'x}. \end{aligned} \quad (15.19)$$

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<sup>7</sup>The ‘classical’ historical example has the ingredients ‘cannon ball’ and ‘snowflake’.

The one-dimensional probability current density is given by (15.6), i.e.  $j = \frac{\hbar}{2mi} (\varphi^* \varphi' - \varphi \varphi'^*)$ . Thus we obtain for the three different partial waves:

$$\begin{aligned} j_{\text{in}} &= -\frac{\hbar}{m} k |B|^2 \\ j_{\text{refl}} &= \frac{\hbar}{m} k \left( \frac{k - k'}{k + k'} \right)^2 |B|^2 \\ j_{\text{trans}} &= -\frac{\hbar}{m} k' \left( \frac{2k}{k + k'} \right)^2 |B|^2. \end{aligned} \quad (15.20)$$

As a measure of the probability that a quantum object is reflected or transmitted, we define the *Transmission* and *Reflection coefficients*:

$$T = \left| \frac{j_{\text{trans}}}{j_{\text{in}}} \right| \quad \text{and} \quad R = \left| \frac{j_{\text{refl}}}{j_{\text{in}}} \right|. \quad (15.21)$$

Intuitively, these expressions indicate the relative proportions of the wavefunction which are transmitted and reflected. Their sum is always 1, since we have ruled out creation and annihilation processes.

For the present example, we obtain the expressions

$$\begin{aligned} T &= \left| \frac{k'}{k} \left( \frac{2k}{k + k'} \right)^2 \right| = \frac{4kk'}{(k + k')^2} \\ R &= \left| \left( \frac{k - k'}{k + k'} \right)^2 \right| = \left( \frac{k - k'}{k + k'} \right)^2. \end{aligned} \quad (15.22)$$

Clearly, because of  $4kk' + (k - k')^2 = 4kk' + k^2 - 2kk' + k'^2 = (k + k')^2$ , we have the relation

$$T + R = 1 \quad (15.23)$$

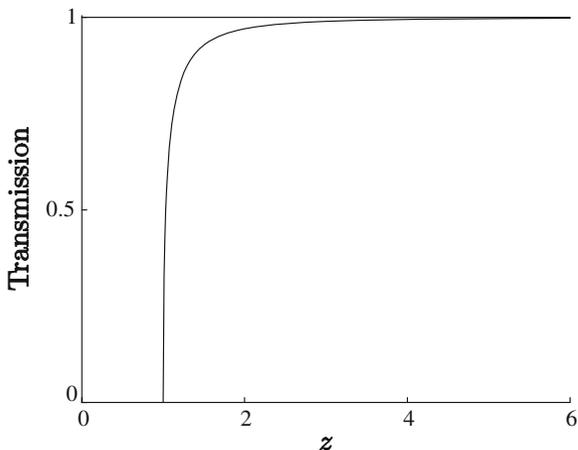
as it indeed must be.

Finally, we investigate how  $T$  and  $R$  behave as functions of  $E$  and  $V_0$  ( $E > V_0$ ). Using the abbreviation  $z = E/V_0$ , and since  $1 < z$  due to  $V_0 < E < \infty$ , we obtain (see Fig. 15.4):

$$T = \frac{4\sqrt{\frac{z-1}{z}}}{\left(1 + \sqrt{\frac{z-1}{z}}\right)^2} = 1 - \frac{1}{16z^2} - \frac{1}{16z^3} - \dots \quad (15.24)$$

$$1 < z = \frac{E}{V_0}; \quad R = 1 - T.$$

**Fig. 15.4** Potential step: transmission coefficient as a function of  $z = E/V_0$



We see the following: if  $E$  is very close to  $V_0$ , then we have  $z \approx 1$ , and hence the transmission coefficient is very small<sup>8</sup> and accordingly the reflection coefficient large. For high energies, we have  $T \rightarrow 1$ ; in this case we have a large transmission coefficient, but always also an (albeit small) portion that is reflected.

### 15.3 Finite Potential Well

This simple example is more realistic than the infinite potential well of Chap. 5, Vol. 1: It allows for bound and free motion. We have a potential of the form (cf. Fig. 15.5):

$$V = \begin{cases} -V_0 & \text{for } -L < x < L; \quad V_0 > 0 \\ 0 & \text{otherwise} \end{cases} \quad (15.25)$$

and thus the three SEq's:

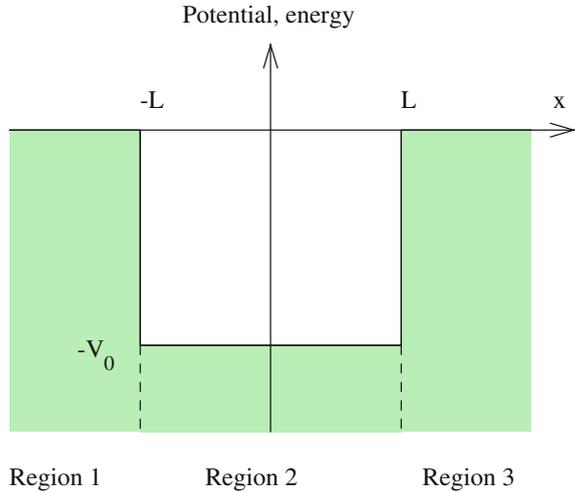
$$\begin{aligned} \text{region 1: } x < -L & \quad E\varphi_1 = -\frac{\hbar^2}{2m}\varphi_1'' \\ \text{region 2: } -L < x < L & \quad E\varphi_2 = -\frac{\hbar^2}{2m}\varphi_2'' - V_0\varphi_2. \\ \text{region 3: } x > L & \quad E\varphi_3 = -\frac{\hbar^2}{2m}\varphi_3'' \end{aligned} \quad (15.26)$$

Depending on the magnitude of  $E$ , we have to make a case distinction: For  $E < 0$ , there are only bound states, while for  $E > 0$  there are only scattering states.<sup>9</sup> In any

<sup>8</sup>In the classical case, we would *always* have transmission 1 for  $E > V_0$ .

<sup>9</sup>This is an example of a spectrum that has both a discrete and a continuous part.

**Fig. 15.5** Finite potential well



case, we can already give the solution in region 2:

$$\text{region 2: } \varphi_2(x) = Be^{ikx} + Ce^{-ikx}; \quad k^2 = \frac{2m}{\hbar^2} (V_0 + E) > 0. \quad (15.27)$$

### 15.3.1 Potential Well, $E < 0$

We first consider energies with  $-V_0 < E < 0$ , that is, bound motion. With

$$\kappa^2 = \frac{2m}{\hbar^2} |E| \quad (15.28)$$

the solutions are

$$\begin{aligned} \text{region 1: } \varphi_1(x) &= Ae^{\kappa x} + A'e^{-\kappa x} \\ \text{region 3: } \varphi_3(x) &= D'e^{\kappa x} + De^{-\kappa x}. \end{aligned} \quad (15.29)$$

Since physically reasonable solutions must be bounded, we must choose  $A' = 0$  and  $D' = 0$ . The other constants are defined by the matching conditions at the two discontinuities.

#### 15.3.1.1 Matching at the Discontinuities

At the discontinuity  $x = -L$  we have the two equations

$$Ae^{-\kappa L} = Be^{-ikL} + Ce^{ikL} \quad \text{and} \quad \kappa Ae^{-\kappa L} = ikBe^{-ikL} - ikCe^{ikL} \quad (15.30)$$

and at the discontinuity  $x = +L$  the two equations

$$De^{-\kappa L} = Be^{ikL} + Ce^{-ikL} \quad \text{and} \quad -\kappa De^{-\kappa L} = ikBe^{ikL} - ikCe^{-ikL}. \quad (15.31)$$

This is a homogeneous system of four equations with four unknowns. In order that the system have non-trivial solutions, the determinant of the coefficient matrix for  $A, B, C, D$  must be equal to zero. Instead of calculating the determinant, we can also multiply the first equation in (15.30) by  $\kappa$  and subtract the two equations. We obtain:

$$0 = \kappa Be^{-ikL} + \kappa Ce^{ikL} - ikBe^{-ikL} + ikCe^{ikL} = (\kappa - ik)e^{-ikL}B + (\kappa + ik)e^{ikL}C \quad (15.32)$$

and analogously from (15.31):

$$0 = \kappa Be^{ikL} + \kappa Ce^{-ikL} + ikBe^{ikL} - ikCe^{-ikL} = (\kappa + ik)e^{ikL}B + (\kappa - ik)e^{-ikL}C. \quad (15.33)$$

With (15.32) and (15.33), we have a homogeneous system for the two unknowns  $B$  and  $C$ . It can be solved if the coefficient determinant for  $B, C$  vanishes, i.e. for

$$(\kappa - ik)^2 e^{-2ikL} - (\kappa + ik)^2 e^{2ikL} \stackrel{!}{=} 0. \quad (15.34)$$

This equation gives the allowed energy values. We insert

$$\kappa \pm ik = \sqrt{\kappa^2 + k^2} e^{\pm i \arctan k/\kappa} \quad (15.35)$$

into (15.34) and obtain

$$\sin\left(2kL + 2 \arctan \frac{k}{\kappa}\right) \stackrel{!}{=} 0. \quad (15.36)$$

The solution is evidently

$$2kL + 2 \arctan \frac{k}{\kappa} \stackrel{!}{=} N\pi; \quad N = 1, 2, 3, \dots \quad (15.37)$$

where  $N$  numbers consecutively the valid solutions in such a way that the smallest energy eigenvalue has the index 1. A closer inspection of this equation is given below; here we will first determine the constants as far as possible. From (15.32) and ((15.33) would give the same information), it follows with (15.35) and because of (15.37) that:

$$\begin{aligned} C &= -B \frac{\kappa - ik}{\kappa + ik} e^{-2ikL} = -B e^{-2i \arctan k/\kappa} e^{-2ikL} \\ &= -B e^{-iN\pi} = B(-1)^{N+1} \end{aligned} \quad (15.38)$$

and thus from (15.30) and (15.31)

$$A = \begin{cases} 2Be^{\kappa L} \cos kL \\ -2iBe^{\kappa L} \sin kL \end{cases} \quad \text{and} \quad D = \begin{cases} 2Be^{\kappa L} \cos kL \\ 2iBe^{\kappa L} \sin kL \end{cases} \quad \text{for } N \begin{matrix} \text{odd} \\ \text{even.} \end{matrix} \quad (15.39)$$

### 15.3.1.2 Energy Eigenvalues

Equation (15.37) is not solvable in closed form. In order to obtain solutions for specific values of  $E$  and  $V_0$ , we must proceed numerically. Nevertheless, we can make general statements with the help of estimates. For this purpose, we rearrange (15.37) as follows:

$$2 \arctan \frac{k}{\kappa} = N\pi - 2kL; \quad N = 1, 2, 3, \dots \quad (15.40)$$

Since  $k$  and  $\kappa$  are positive, we can estimate

$$0 < 2 \arctan \frac{k}{\kappa} < \pi. \quad (15.41)$$

Thus we obtain the inequality

$$0 < N\pi - 2kL < \pi \quad \text{or} \quad (N-1)\pi < 2kL < N\pi. \quad (15.42)$$

Since there are no negative terms, we can square. Substituting  $k^2 = 2m(V_0 - |E|)/\hbar^2$  and subsequent rearranging yields

$$V_0 - \frac{\hbar^2}{2m} \left( \frac{N}{2L}\pi \right)^2 < |E| < V_0 - \frac{\hbar^2}{2m} \left( \frac{N-1}{2L}\pi \right)^2. \quad (15.43)$$

This equation allows us to draw several conclusions:

1. For  $N = 1$  we have

$$V_0 - \frac{\hbar^2}{2m} \left( \frac{\pi}{2L} \right)^2 < |E| < V_0. \quad (15.44)$$

It follows that there is always a solution. As we shall see below, it is symmetrical. This ‘lowest’ solution is also called the *ground state*.

2. For  $N = 2$ , we have

$$V_0 - \frac{\hbar^2}{2m} \left( \frac{2\pi}{2L} \right)^2 < |E| < V_0 - \frac{\hbar^2}{2m} \left( \frac{\pi}{2L} \right)^2. \quad (15.45)$$

It follows that there is a second state (the *first excited state*), if  $V_0 > \frac{\hbar^2}{2m} \left( \frac{\pi}{2L} \right)^2$ . As we shall see below, this state is antisymmetric.

3. Similarly, one sees that the  $N$ -th state exists if  $V_0 > \frac{\hbar^2}{2m} \left( \frac{N-1}{2L} \pi \right)^2$ .

4. There is an  $N_0$ , from which onwards the right side of the inequality is no longer satisfied. It follows that in each potential well of the kind we are considering, there is only a finite number of energy levels (see exercises).

### 15.3.1.3 Eigenfunctions

We now know that there is a finite number of solutions of the (15.36). We number them from 1 to  $N_0$  (since  $k$  and  $\kappa$  depend on  $E$ , they also depend on  $N$ , which is indicated by a corresponding index). For each of these solutions, there is an eigenfunction; we distinguish these according to the parity of the energy quantum number  $N$ . With (15.38) and (15.39), it follows that

$$\begin{aligned}\varphi_{1,N}(x) &= 2B e^{\kappa_N L} \cos k_N L \cdot e^{\kappa_N x} \\ \varphi_{2,N}(x) &= 2B \cdot \cos k_N x && \text{for } N \text{ odd} \\ \varphi_{3,N}(x) &= 2B e^{\kappa_N L} \cos k_N L \cdot e^{-\kappa_N x}\end{aligned}\tag{15.46}$$

and

$$\begin{aligned}\varphi_{1,N}(x) &= -2i B e^{\kappa_N L} \sin k_N L \cdot e^{\kappa_N x} \\ \varphi_{2,N}(x) &= 2i B \cdot \sin k_N x && \text{for } N \text{ even.} \\ \varphi_{3,N}(x) &= 2i B e^{\kappa_N L} \sin k_N L \cdot e^{-\kappa_N x}\end{aligned}\tag{15.47}$$

The solutions in region 2, i.e. within the potential well, are evidently standing waves. The parity of the eigenfunctions alternates on climbing up the ‘energy ladder’, with the ground state symmetric. By the way, this parity property is a consequence of the symmetry of the problem.

## 15.3.2 Potential Well, $E > 0$

We now consider the case  $E > 0$ , i.e. free motion. With

$$k'^2 = \frac{2m}{\hbar^2} E\tag{15.48}$$

the solutions read

$$\begin{aligned}\text{region 1: } \varphi_1(x) &= A' e^{ik'x} + A e^{-ik'x} \\ \text{region 3: } \varphi_3(x) &= D e^{ik'x} + F e^{-ik'x}\end{aligned}\tag{15.49}$$

and from above we have

$$\text{region 2: } \varphi_2(x) = B e^{ikx} + C e^{-ikx}.\tag{15.50}$$

If we require that the incoming wave of amplitude  $F$  is incident on the potential well from the right, we have  $A' = 0$ , because in region 1, a wave coming from the left cannot be present. To determine the other constants, we use the matching conditions at the two discontinuities. They are

$$\begin{aligned} Ae^{ik'L} &= Be^{-ikL} + Ce^{ikL} \\ -k'Ae^{ik'L} &= kB e^{-ikL} - kC e^{ikL} \end{aligned} \quad (15.51)$$

and

$$\begin{aligned} Be^{ikL} + Ce^{-ikL} &= De^{ik'L} + Fe^{-ik'L} \\ kB e^{ikL} - kC e^{-ikL} &= k'D e^{ik'L} - k'F e^{-ik'L}. \end{aligned} \quad (15.52)$$

These are four equations for four unknowns (the amplitude  $F$  can be chosen at will). Their solution reads

$$\begin{aligned} A &= \frac{-4k'k}{N} e^{-2ik'L} F \\ B &= \frac{2k'(k' - k)}{N} e^{ikL} e^{-ik'L} F \\ C &= -\frac{2k'(k' + k)}{N} e^{-ikL} e^{-ik'L} F \\ D &= \frac{2i \sin(2kL)(k'^2 - k^2)}{N} e^{-2ik'L} F \end{aligned} \quad (15.53)$$

with

$$\begin{aligned} N &= e^{2ikL}(k' - k)^2 - e^{-2ikL}(k' + k)^2 \\ &= 2i(k'^2 + k^2) \sin(2kL) - 4kk' \cos(2kL). \end{aligned} \quad (15.54)$$

The transmission and reflection coefficients are given by

$$T = \frac{|A|^2}{|F|^2} \quad \text{and} \quad R = \frac{|D|^2}{|F|^2} \quad (15.55)$$

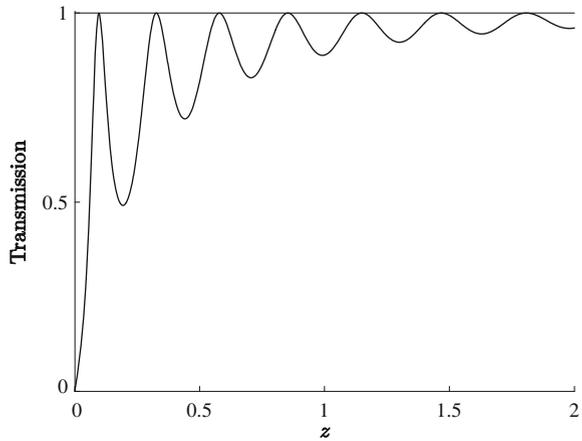
and this leads to

$$T = \frac{16k'^2 k^2}{|N|^2} \quad \text{and} \quad R = \frac{2(k'^2 - k^2)(1 - \cos(4kL))}{|N|^2} = 1 - T \quad (15.56)$$

with

$$|N|^2 = 2k'^4 + 12k'^2 k^2 + 2k^4 - 2(k'^2 - k^2)^2 \cos(4kL). \quad (15.57)$$

**Fig. 15.6** Transmission coefficient (15.60) for scattering by the potential well with  $\mu = 15$  as a function of  $z = \frac{E}{V_0}$



Because of

$$k'^2 = \frac{2m}{\hbar^2}E \quad \text{and} \quad k^2 = \frac{2m}{\hbar^2}(E + V_0) \tag{15.58}$$

and with

$$z = \frac{E}{V_0}; \quad \mu = \sqrt{\frac{2m}{\hbar^2}V_0L^2}, \tag{15.59}$$

it follows for the transmission coefficient:

$$T = \frac{z(z+1)}{z(z+1) + \frac{1-\cos 4kL}{8}} = \frac{z(z+1)}{z(z+1) + \frac{1-\cos 4\mu\sqrt{z+1}}{8}}. \tag{15.60}$$

We see that  $T = 1$  for  $\cos 4kL = 1$ , which means that  $4kL = 2m\pi$ . With  $\lambda = \frac{2\pi}{k}$ , the intuitively-clear condition  $m\frac{\lambda}{2} = 2L$  follows, i.e. a kind of resonance condition, as is seen very nicely in Fig. 15.6.

### 15.4 Potential Barrier, Tunnel Effect

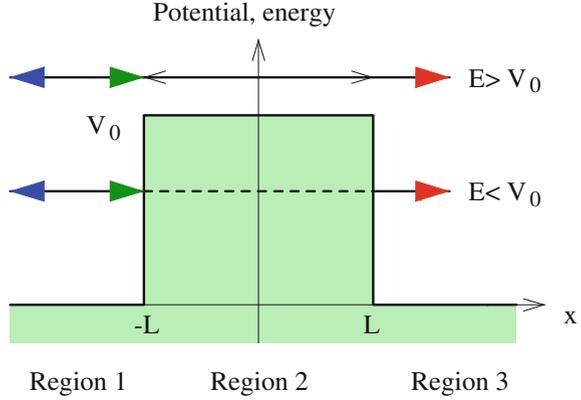
The potential is given by (cf. Fig. 15.7):

$$V = \begin{cases} V_0 & \text{for } -L < x < L; \quad V_0 > 0 \\ 0 & \text{otherwise.} \end{cases} \tag{15.61}$$

In view of the description of scattering processes, this potential is more realistic than the infinite potential step. However, the computational effort is also significantly greater.

The solutions in the different regions are

**Fig. 15.7** Potential barrier.  
*Straight lines: oscillation,  
 broken line: exponential.  
 Incoming green, reflected  
 blue, transmitted red*



$$\begin{aligned}
 x < -L: & \quad \varphi_1(x) = Ae^{ikx} + Be^{-ikx} \\
 -L < x < L: & \quad \varphi_2(x) = Ce^{\gamma x} + De^{-\gamma x} \\
 x > L: & \quad \varphi_3(x) = Fe^{ikx} + Ge^{-ikx}
 \end{aligned} \tag{15.62}$$

with  $k^2 = \frac{2m}{\hbar^2}E$ . We can consider the cases  $E > V_0$  and  $E < V_0$  simultaneously by defining

$$\gamma = \begin{cases} \kappa & \text{for } E < V_0 \\ ik' & \text{for } E > V_0 \end{cases} \quad \text{with} \quad \begin{cases} \kappa^2 = \frac{2m}{\hbar^2}(V_0 - E) \\ k'^2 = \frac{2m}{\hbar^2}(E - V_0). \end{cases} \tag{15.63}$$

For a change, we assume this time that the incident wave comes from the left and has amplitude  $A$ . Then in region 3, there is no wave running from the right to the left, which means that  $G = 0$ . At the discontinuities  $x = \pm L$ , we have

$$\begin{aligned}
 Ae^{-ikL} + Be^{ikL} &= Ce^{-\gamma L} + De^{\gamma L} \\
 ikAe^{-ikL} - ikBe^{ikL} &= \gamma Ce^{-\gamma L} - \gamma De^{\gamma L}
 \end{aligned} \tag{15.64}$$

and

$$\begin{aligned}
 Ce^{\gamma L} + De^{-\gamma L} &= Fe^{ikL} \\
 \gamma Ce^{\gamma L} - \gamma De^{-\gamma L} &= ikFe^{ikL}.
 \end{aligned} \tag{15.65}$$

The calculation of the constants as multiples of  $A$  is given in Appendix X, Vol. 2.

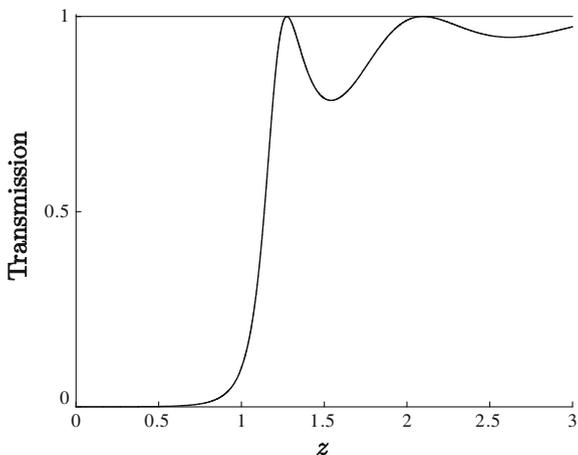
The partial waves of interest to us are

$$\varphi_{\text{in}} = Ae^{ikx}; \quad \varphi_{\text{refl}} = Be^{-ikx}; \quad \varphi_{\text{trans}} = Fe^{ikx}. \tag{15.66}$$

Transmission and reflection coefficients are given by

$$T = \frac{|F|^2}{|A|^2}; \quad R = \frac{|B|^2}{|A|^2}. \tag{15.67}$$

**Fig. 15.8** Potential barrier: transmission coefficient as a function of  $z = E/V_0$  for  $\mu = 3$



We confine the discussion to  $T$ . The somewhat lengthy calculation is given in Appendix X, Vol. 2. With

$$z = \frac{E}{V_0}; \quad k'L = \mu\sqrt{z-1}; \quad \kappa L = \mu\sqrt{1-z}; \quad \mu = \sqrt{\frac{2m}{\hbar^2} V_0 L^2}, \quad (15.68)$$

the result reads<sup>10</sup>:

$$T = \begin{cases} \frac{8z(z-1)}{8z(z-1) + 1 - \cosh 4\kappa L} = \frac{z(z-1)}{z(z-1) + \frac{1 - \cosh 4\mu\sqrt{1-z}}{8}} & \text{for } E < V_0; \quad 0 < z < 1 \\ \frac{8z(z-1)}{8z(z-1) + 1 - \cos 4k'L} = \frac{z(z-1)}{z(z-1) + \frac{1 - \cos 4\mu\sqrt{z-1}}{8}} & \text{for } E > V_0; \quad z > 1. \end{cases} \quad (15.69)$$

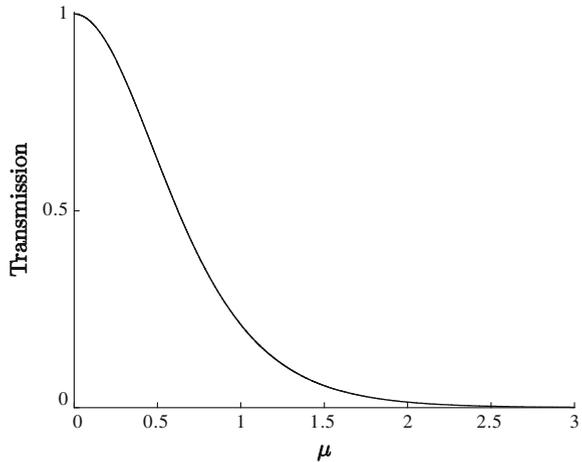
In Fig. 15.8, the transmission coefficient is shown as a function of  $z = E/V_0$ . We see that in the range  $0 < z \leq 1$ , it *always* holds that  $T > 0$ .

This means that we always have a part of the wavefunction which ‘tunnels through’, i.e. shows a behavior which is impossible in classical mechanics. The tunneling probability decreases of course with increasing width of the potential barrier. We illustrate this in Fig. 15.9 for the case  $E = V_0/2$ . This sensitive dependence of the tunneling on the potential width is responsible e.g. for the wide range of decay times observed for  $\alpha$  decay; technically, it is used in tunnel diodes.

For  $E = V_0$ , we also find both reflected and transmitted components, because of

<sup>10</sup>Because of  $\cosh iy = \cos y$  or  $\cos iy = \cosh y$ , one of the two expressions for  $T$  is in fact sufficient for real  $y$ .

**Fig. 15.9** Transmission coefficient for  $E = V_0/2$  as a function of  $\mu \sim L$



$$T(z=1) = \frac{1}{1 + \mu^2}. \quad (15.70)$$

This is also true for all values  $z > 1$ , but with isolated exceptions, since for

$$z = z_m = 1 + \left(\frac{m\pi}{2\mu}\right)^2; \quad m = 1, 2, \dots \rightarrow T(z_m) = 1, \quad (15.71)$$

there are only transmitted and no reflected components.

Apart from the values  $E = \left[1 + \left(\frac{m\pi}{2\mu}\right)^2\right] V_0$ , for  $0 < z < \infty$  we *always* obtain both reflected and transmitted portions of the wavefunction in the case of the potential barrier. For very large values of the energy, the reflection probability is indeed very small, but it is not zero, i.e. it exists in principle. In contrast, in classical mechanics we have either reflection ( $E < V_0$ ) or transmission ( $E > V_0$ ).

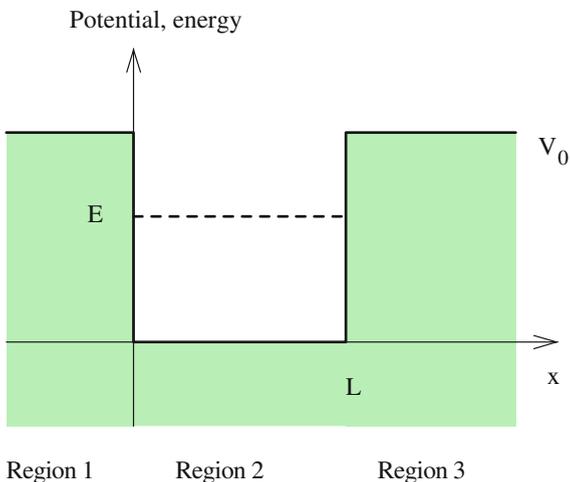
## 15.5 From the Finite to the Infinite Potential Well

In considering the infinite potential well, we assumed that the wavefunction vanishes at the potential walls. We want now to justify that assumption.

We start with a finite potential well (see Fig. 15.10):

$$V = \begin{cases} 0 & \text{for } 0 < x < L \\ V_0 > 0 & \text{otherwise.} \end{cases} \quad (15.72)$$

**Fig. 15.10** Potential well for the discussion of the limit  $V_0 \rightarrow \infty$



We calculate the bound solutions and let then go  $V_0$  to infinity. We have for the stationary SEq (region 3 is not required for the following consideration):

$$E\varphi_1 = -\frac{\hbar^2}{2m}\varphi_1'' + V_0\varphi_1 \text{ for } x < 0; \quad E\varphi_2 = -\frac{\hbar^2}{2m}\varphi_2'' \text{ for } 0 < x < L \quad (15.73)$$

or

$$\varphi_1'' = \frac{2m}{\hbar^2}(V_0 - E)\varphi_1 = \kappa^2\varphi_1; \quad \varphi_2'' = -\frac{2m}{\hbar^2}E\varphi_2 = -k^2\varphi_2. \quad (15.74)$$

It follows that:

$$\begin{aligned} \varphi_1(x) &= Ae^{\kappa x}; & \varphi_2(x) &= Be^{ikx} + Ce^{-ikx} \\ \varphi_1'(x) &= \kappa Ae^{\kappa x}; & \varphi_2'(x) &= ikBe^{ikx} - ikCe^{-ikx}. \end{aligned} \quad (15.75)$$

At  $x = 0$ , we have

$$A = B + C; \quad \kappa A = ikB - ikC. \quad (15.76)$$

From these two equations, we find:

$$C = -\frac{\kappa - ik}{\kappa + ik}B \quad (15.77)$$

and therefore

$$A = B + C = \frac{2ik}{\kappa + ik}B. \quad (15.78)$$

The limit  $V_0 \rightarrow \infty$  means  $\kappa \rightarrow \infty$  (while  $k$  remains fixed). Hence it follows that  $A \rightarrow 0$ . In this way, we have justified in retrospect our *ansatz*  $\varphi_1(0) = 0$  at the discontinuity of the infinite potential well. For the wavefunction in region 2, we have

$$\begin{aligned}\varphi_2(0) &= B + C = \frac{2ik}{\kappa + ik} B \\ \varphi_2'(0) &= ikB - ikC = \frac{2ik\kappa}{\kappa + ik} B\end{aligned}\quad (15.79)$$

and for  $V_0 \rightarrow \infty$  it follows, as it indeed must:

$$\varphi_2(0) \rightarrow 0; \quad \varphi_2'(0) \rightarrow 2ikB. \quad (15.80)$$

## 15.6 Wave Packets

We have already discussed several times the fact that a plane wave cannot describe a physical object because it has the same magnitude for all positions and times. But in spite of this, it is common practice to work with this handy formulation, as we know. This is due to the linearity of the SEq and the consequent superposability of its solutions. It allows us to overlay plane waves in such a way that a physically meaningful expression results.

We want to carry this out as an example for the potential step discussed above: There is an incoming wave in the region  $x > 0$ , incident from the right, a transmitted wave from the right to the left in  $x < 0$  and a reflected wave from the left to the right in  $x > 0$ . With

$$k_0 = \sqrt{\frac{2m}{\hbar^2} V_0}; \quad \gamma(k) = \begin{cases} \kappa = \sqrt{k_0^2 - k^2} \\ -ik' = -i\sqrt{k^2 - k_0^2} \end{cases} \quad \text{for } \begin{matrix} E < V_0 \text{ or } k < k_0, \\ E > V_0 \text{ or } k > k_0, \end{matrix} \quad (15.81)$$

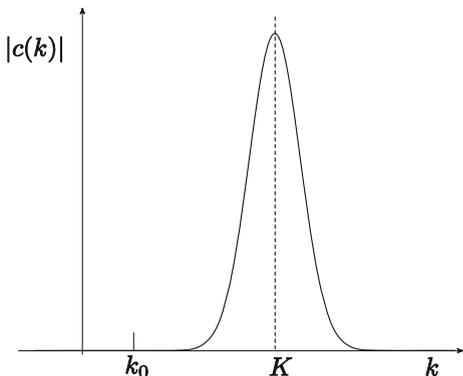
we can write the solutions for fixed  $k > 0$  as

$$\varphi_1 = ce^{-ikx} + c \frac{ik + \gamma}{ik - \gamma} e^{ikx}; \quad \varphi_2 = c \frac{2ik}{ik - \gamma} e^{\gamma x}. \quad (15.82)$$

We obtain a total solution by integrating over the continuous index  $k > 0$ . With  $\omega = \frac{\hbar k^2}{2m}$ , it follows that

$$\begin{aligned}\Psi_1(x, t) &= \int_0^\infty c(k) \left( e^{-ikx} + \frac{ik + \gamma}{ik - \gamma} e^{ikx} \right) e^{-i\omega t} dk \\ \Psi_2(x, t) &= \int_0^\infty c(k) \frac{2ik}{ik - \gamma} e^{\gamma x} e^{-i\omega t} dk\end{aligned}\quad (15.83)$$

**Fig. 15.11** Schematic representation of the amplitude function  $|c(k)|$  for comparison with the classical transmission



where  $c(k)$  is an arbitrary function of  $k$ . With suitable  $c(k)$ , one can generate rather complicated wavefunctions. We confine ourselves to a situation that allows comparison with classical behavior (either reflection or transmission). We choose transmission.<sup>11</sup> From the classical perspective, this case corresponds to an object that travels from the right to the left with momentum  $P$  towards the potential step, and from there continues in the same direction, but with a smaller momentum  $P'$ .

Since the classical particle has a definite momentum  $P = \hbar K$ , we choose for  $c(k)$  a function that has a sharp maximum at  $k = K$ , has nonvanishing values only in a neighborhood of  $K$ , and (for the sake of simplicity) vanishes identically for  $k \leq k_0$ ; see Fig. 15.11.<sup>12</sup>

Thus we can write<sup>13</sup>

$$\begin{aligned} \Psi_1(x, t) &= \int_{k_0}^{\infty} c(k) e^{-i(kx + \omega t)} dk + \int_{k_0}^{\infty} c(k) \frac{k - k'}{k + k'} e^{i(kx - \omega t)} dk = \Psi_{\text{in}} + \Psi_{\text{refl}} \\ \Psi_2(x, t) &= \int_{k_0}^{\infty} c(k) \frac{2k}{k + k'} e^{-i(k'x + \omega t)} dk = \Psi_{\text{trans}}. \end{aligned} \tag{15.84}$$

We immediately see that we again have three types of waves<sup>14</sup>: incoming, reflected, and transmitted, and that—in contrast to classical mechanics—there is *always* a reflected wave.<sup>15</sup>

Even for very simple distributions  $c(k)$ , it is not possible to perform the integrations in closed form.<sup>16</sup> But we can make the following general observation: the magnitude of the integrals in (15.84) depends essentially on how fast the exponential

<sup>11</sup>More on wave packets can be found in Appendix D, Vol. 2.

<sup>12</sup>If we call  $\Delta k$  the width of the function, then  $\Delta k \ll K$  must apply.

<sup>13</sup>Due to  $c(k) = 0$ .

<sup>14</sup>We note that these are ‘true’ waves, functions of time and space.

<sup>15</sup>We recall the quantum-mechanical truck that bounces off a mosquito flying against its windshield.

<sup>16</sup>If  $c(k)$  is given by a Gaussian curve, at least the term  $\Psi_{\text{in}}$  can be calculated; see Chap. 5, Vol. 1 and Appendix D, Vol. 2.

functions oscillate in the neighborhood of  $K$ —the faster, the smaller the integral (or its absolute value). This is due to the fact that with a faster oscillation, the areas above the  $k$  axis are better compensated by areas of opposite sign. In general, we find the biggest contribution if the exponent does not vary in the neighborhood of  $K$ ; that is, if its derivative with respect to  $k$  vanishes.<sup>17</sup> This means, for example for the incoming wave,

$$\frac{d}{dk} (kx + \omega t) \Big|_{k=K} = x + \frac{\hbar K}{m} t = 0. \quad (15.85)$$

Thus, the incoming wave packet is particularly large for  $x$  values near  $x = -\frac{\hbar K}{m} t$ , and this peak moves with the *group velocity*  $v_g = -\frac{\hbar K}{m}$ . Accordingly, for the reflected wave we have the group velocity  $v_g = \frac{\hbar K}{m}$ . The value of  $v_g$  is obtained in both cases as  $v_g = \frac{d\omega}{dk}$ , which is the usual definition of group velocity, while the phase velocity  $v_{ph}$  (i.e. the propagation velocity of a wave component with a well-defined oscillation frequency) is given by  $v_{ph} = \frac{\omega}{k}$ . We consider the transmitted wave. The stationarity of the phase

$$\frac{d}{dk} (k'x + \omega t) \Big|_{k=K} = 0 \quad (15.86)$$

gives

$$x + \frac{\hbar K'}{m} t = 0; \quad K' = \sqrt{K^2 - \frac{2m}{\hbar^2} V_0}; \quad v_g = \frac{d\omega}{dk} \Big|_{k=K'}. \quad (15.87)$$

We have a stationary phase only in the following cases: (a)  $\Psi_{in}$  for  $t < 0$  and  $x > 0$ ; (b)  $\Psi_{refl}$  for  $t > 0$  and  $x > 0$ ; (c)  $\Psi_{trans}$  for  $t > 0$  and  $x < 0$ . This means that at large negative times, only the incident wave packet provides a significant contribution; at  $t \approx 0$ , all three sub-packets exist with similar amplitudes; at large positive times, only the reflected and transmitted wave packets provide significant contributions. In other words: At  $t \ll 0$  we have an incoming (from the right to the left) wave packet; at  $t \approx 0$  there is a confusing ‘wriggling’, and at  $t \gg 0$  we again have a clear-cut situation, namely for  $x > 0$  a reflected (running to the right) and for  $x < 0$  a transmitted (running to the left) wave packet.<sup>18</sup>

Finally, we want to address very briefly problems which may arise in explaining these relationships to laypeople, whether in schools or elsewhere. First, we have already pointed out that terms such as ‘incoming wave’ require bearing in mind tacitly the factor  $e^{-i\omega t}$ . Without this factor, the name would be misleading, because  $e^{ikx}$  is not a wave travelling anywhere, but simply a time-independent spatial oscillation. In general, these facts are not considered in school classes; in addition, complex numbers

<sup>17</sup>This is why the procedure is also called the method of stationary phase.

<sup>18</sup>We recall that the wavefunction does not describe the object itself, but rather allows the calculation of probabilities for observing it at a particular location.

are nearly always avoided. Thus, one has to argue ‘somehow’ that e.g.  $\cos kx$  is an incoming wave.

Another problem in this context: Teaching and learning software illustrate e.g. scattering by the potential step, but of course do this with wave packets of the form (15.83); with plane waves, one would see not too much. However, wave packets and similar formulations are usually not taught at all in school classes, so it seems difficult to establish the relationship between the mathematics and computer simulation results.

## 15.7 Exercises

1. Given the potential step

$$V(x) = \begin{cases} 0 & \text{for } x > 0 \\ V_0 > 0 & \text{for } x \leq 0. \end{cases} \quad (15.88)$$

The incident quantum object is described as a plane wave running from the right to the left with  $E > V_0$ . Determine the transmission and reflection coefficients.

2. Given a finite potential well of depth  $V_0$  and width  $L$ ; estimate the number of energy levels.
3. Given a delta potential at  $x = 0$ ; determine the spectrum (negative potential,  $E < 0$ ) and the situation for scattering (positive potential,  $E > 0$ ).
4. Given the potential barrier

$$V(x) = \begin{cases} V_0 > 0 & \text{for } -L < x < L \\ 0 & \text{otherwise.} \end{cases} \quad (15.89)$$

The incident quantum object is described by a plane wave running from the left to the right. Determine the transmission and reflection coefficients.

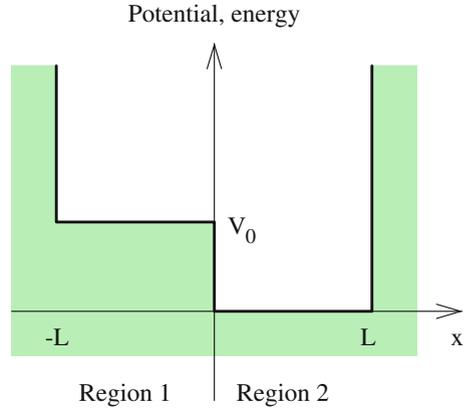
5. Given the one-sided infinite potential well

$$V(x) = \begin{cases} 0 & L < x \\ -V_0 & \text{for } 0 < x \leq L \\ \infty & x \leq 0 \end{cases} \quad (15.90)$$

with  $V_0 > 0$ . For the energy, let  $-V_0 < E < 0$ . Sketch the potential. Determine the stationary SEq in the different regions and deduce from them an *ansatz* for the wavefunction. Adjust the wavefunctions at the discontinuities and show that the allowed energy levels are defined by the equation  $k \cot kL = -\kappa$  with  $k^2 = 2m(V_0 + E)/\hbar^2$  and  $\kappa^2 = -2mE/\hbar^2$ . Is there always (i.e. for all  $V_0$ ) a bound state?

6. Given the potential

**Fig. 15.12** The potential of (15.92)



$$V(x) = \begin{cases} \infty & x < 0 \\ V_0 > 0 & \text{for } 0 \leq x \leq L. \\ 0 & L < x \end{cases} \quad (15.91)$$

An object described by a plane wave passes from the right to the origin. Sketch the potential. Calculate the wavefunction for the case  $E < V_0$ . Which regions are classically allowed, which are not? Determine first the stationary SEq's in the different regions and solve them with an appropriate *ansatz*. Are all the mathematical solutions physically allowed? Determine the free constants using the continuity conditions at the discontinuities of the potential.

Perform the calculations for the case  $E > V_0$ , also.

7. Given a potential step embedded in an infinite potential well (see Fig. 15.12):

$$V(x) = \begin{cases} 0 & 0 < x < L \\ V_0 > 0 & \text{for } -L < x \leq 0. \\ \infty & x \geq |L| \end{cases} \quad (15.92)$$

Calculate the spectrum for  $E > V_0$ .

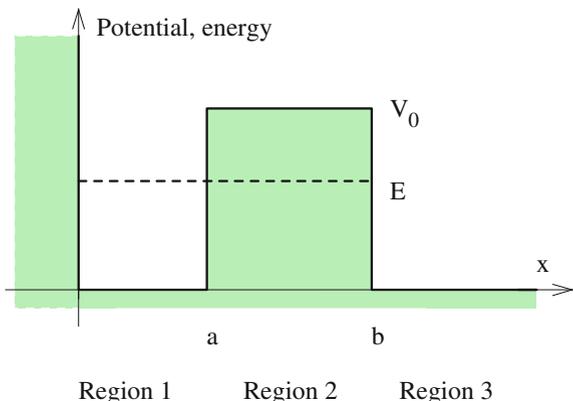
8. (Resonances) Given a potential barrier in front of an infinite potential wall (see Fig. 15.13):

$$V(x) = \begin{cases} \infty & x < 0 \\ V_0 > 0 & \text{for } \leq x \leq b. \\ 0 & \text{otherwise} \end{cases} \quad (15.93)$$

The incident quantum object has the energy  $E < V_0$  and comes from the right. For which parameter values is the phase shift of the outgoing wave particularly large/does the phase change especially fast? What is the physical explanation?

9. In this chapter, a transcendental equation of the form

**Fig. 15.13** The potential of (15.93)



$$\tan kd = -\frac{k}{\kappa} = \quad ; \quad \kappa = \sqrt{\kappa_V^2 - k^2} \quad ; \quad k < \kappa_V \quad (15.94)$$

occurs several times. Find an approximate solution for large  $d$ .

10. Given the double well potential:

$$\begin{aligned} \text{region 1: } & -L \leq x \leq -a \quad V = 0 \\ \text{region 2: } & -a < x < a \quad V = V_0 > 0. \\ \text{region 3: } & a \leq x \leq L \quad V = 0 \end{aligned} \quad (15.95)$$

$V$  is infinite for  $|x| > L$ . We consider only energies  $E$  for which  $E < V_0$ .

- (a) Due to the symmetry of the problem ( $H(x) = H(-x)$ ), there are symmetric and antisymmetric eigenfunctions,  $sS$  and  $aS$  (cf. Chap. 21, Vol. 2). Determine these functions and their eigenvalue equations.
- (b) Show that there is no solution of the eigenvalue equations below a certain threshold value of  $V_0$ .
- (c) Show that the ground state is symmetric.
- (d) Solve the eigenvalue equations approximately for the case of a ‘thick’ barrier, i.e. for very large  $a$ .
- (e) The initial state is assumed to be a linear combination of the symmetric and the antisymmetric states of the same order (for the sake of simplicity with equal amplitudes,  $A_s = A_a = A$ ). Determine the time behavior of the wavefunction. Calculate the probabilities  $P_i(t)$  of finding the object in region  $i$ .
- (f) In the case of a thick barrier, it holds that  $k_a - k_s \ll k_a + k_s$ . Calculate up to and including quadratic terms in  $k_a - k_s$  the quantities  $R_{\max}^{\min} = \min(P_3) / \max(P_3)$  and  $\Delta\omega$ . Discuss your findings.
- (g) In the ammonia molecule  $NH_3$ , the  $N$  atom tunnels back and forth through the plane of the three  $H$  atoms. This situation can be modelled by the double well potential with parameters  $a = 0.2 \cdot 10^{-10}$  m,  $d = 0.3 \cdot 10^{-10}$  m,  $V_0 = 0.255$  eV and  $m = 4 \cdot 10^{-27}$  kg (the reduced mass is  $\frac{3m_H m_N}{3m_H + m_N}$ ).

Compute numerical values for the ground-state levels, the frequency and  $R_{\max}^{\min}$ . Discuss your findings.

11. For an illustration of the method of stationary phase, consider the (unnormalized) wavefunction

$$\psi(x, t) = \int_{-\infty}^{\infty} |A(k)| e^{i\varphi(k)} e^{i(kx - \omega t)} dk \quad (15.96)$$

with

$$\omega = ck; \quad \varphi(k) = -x_0 k \quad (15.97)$$

and

$$|A(k)| = \begin{cases} \kappa^2 - (k - K)^2 & \text{for } 0 < K - \kappa \leq k \leq K + \kappa \\ 0 & \text{otherwise} \end{cases}. \quad (15.98)$$

The constants  $\kappa$ ,  $K$  and  $x_0$  are positive. Calculate explicitly  $\psi(x, t)$  and discuss its properties. What is the physical significance of  $x_0$ ?