V. (4) Scattering from a Step Potential

A typical step potential is shown in Fig. IV. 4.1.

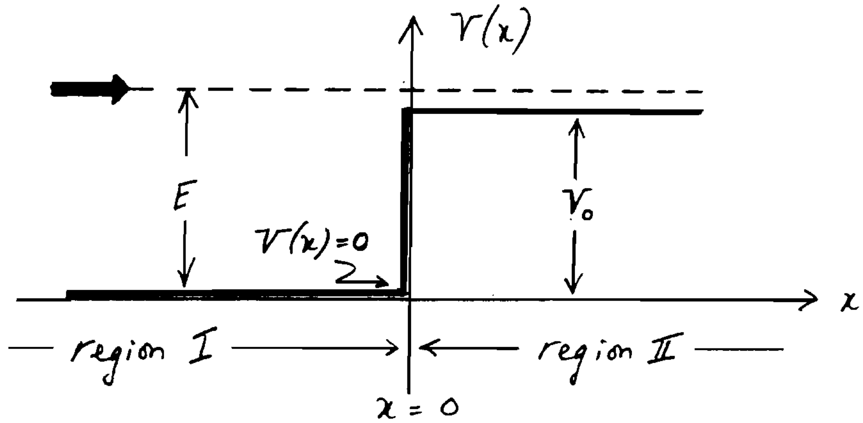

Fig. IV. 4.1. A step potential of height V_0. The dashed line symbolizes the energies of particles in a beam incident from the left.

We consider a beam of particles incident on the step from the left. Each particle has kinetic energy E. We treat this problem as a steady-state problem in that the beam can be viewed as "flowing" continuously and not changing its properties with time. Thus, we apply the time-independent Schrödinger equation to the problem

With reference to Fig. IV. 4.1, the time-independent Schrödinger equation for region I is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\,\psi(x), \qquad (4.1)$$

and for region II is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x). \qquad (4.2)$$

$\boxed{\text{CASE I : } E > V_0}$

Equations (4.1) and (4.2) can each be written in the form of eq. (2.3) and, thus, their solutions can be written in the form of eq. (2.6), i.e. for region I

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}, \qquad (4.3)$$

and for region II

$$\psi_{II}(x) = Ce^{ik_2x} + De^{-ik_2x}; \qquad (4.4)$$

where

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad \text{(real and positive)} \qquad (4.5)$$

and

$$k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}, \quad \text{(real and positive)}, \qquad (4.6)$$

and A, B, C, and D are (complex) constants.

The solutions to Schrödinger's equation are required to obey the <u>continuity conditions</u> (see box on next page) at the boundaries of each region -- in the present case the boundary between region I and region II -- thus at $x=0$,

$$\psi_I(x=0) = \psi_{II}(x=0), \qquad (4.7)$$

$$\therefore Ae^{ik_1 0} + Be^{-ik_1 0} = Ce^{ik_2 0} + De^{-ik_2 0}, \qquad (4.8)$$

$$\therefore \quad A + B = C + D, \qquad (4.9)$$

and

$$\left.\frac{d\psi_I(x)}{dx}\right)_{x=0} = \left.\frac{d\psi_{II}(x)}{dx}\right)_{x=0}, \tag{4.10}$$

$$\therefore \quad ik_1 A e^{ik_1x} - ik_1 B e^{-ik_1x} = \left. ik_2 C e^{ik_2x} - ik_2 D e^{-ik_2x} \right)_{x=0}, \tag{4.11}$$

$$\therefore \quad k_1(A-B) = k_2(C-D). \tag{4.12}$$

<u>Continuity Conditions for Wave Functions</u>

(i). Continuity of $\psi(x)$:

The wave function, $\psi(x)$, is interpreted to be a probability amplitude. For this to be meaningful, $\psi(x)$ must be a <u>single-valued function</u>. Thus, at a boundary, say $x=a$, between two regions I and II, $\psi_I(x)$ and $\psi_{II}(x)$ must obey

$$\psi_I(x=a) = \psi_{II}(x=a)$$

(ii). Continuity of $\psi'(x)$:

The wave function, $\psi(x)$ must obey Schrödinger's equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

for all values of x. If $\psi'(x)$ is discontinuous anywhere, then $\psi''(x)$ would be infinite at the discontinuity and thus E would be infinite (for a finite $V(x)$). Thus, at a boundary, $x=a$, between regions I and II,

$$\left.\psi_I'(x)\right)_{x=a} = \left.\psi_{II}'(x)\right)_{x=a}$$

‡ If A, B, and C are complex, this is a system of four equations in six unknowns.

A simplification is possible for region I: because the beam is incident from the left, the term De^{-ik_2x} must vanish, i.e. $D = 0$. This ensures that there is no component of $\psi_{II}(x)$ with negative wave number and hence negative momentum (recall $p = k\hbar$). Thus, our task is to solve the simultaneous equations

$$A + B = C, \tag{4.13}$$

and

$$k_1(A - B) = k_2 C. \tag{4.14}$$

Equations (4.13) and (4.14) form a system of two equations in three unknowns‡, A, B and C. The amplitude A is related to the intensity of the incident beam (the term e^{ik_1x} in region I), the amplitude B is related to the intensity of the reflected beam (the term e^{-ik_1x} in region I), and the amplitude C is related to the intensity of the transmitted beam (the term e^{ik_2x} in region II). We proceed by obtaining expressions for B and C in terms of A. Thus, multiplying eq. (4.13) by k_1 and: adding to eq. (4.14), we obtain

$$2k_1 A = (k_1 + k_2) C; \tag{4.15}$$

subtracting eq. (4.14), we obtain

$$2k_1 B = (k_1 - k_2) C. \tag{4.16}$$

Therefore,

$$C = \frac{2k_1}{k_1 + k_2} A, \tag{4.17}$$

and from eqs. (4.16) and (4.17)

$$B = \frac{(k_1 - k_2)}{2k_1} \frac{2k_1}{(k_1 + k_2)} A, \tag{4.18}$$

$$\therefore \quad B = \left(\frac{k_1 - k_2}{k_1 + k_2} \right) A. \tag{4.19}$$

We define the <u>flux</u> or <u>current</u> to be given by

flux or current ≡ (probability of having velocity v)× (velocity, v). (4.20)

Then we have:

$$\text{incident flux} = |A|^2 \frac{k_1 \hbar}{m} \equiv I, \tag{4.21}$$

$$\text{reflected flux} = |B|^2 \frac{k_1 \hbar}{m} \equiv R, \tag{4.22}$$

$$\text{transmitted flux} = |C|^2 \frac{k_2 \hbar}{m} \equiv T. \tag{4.23}$$

Note that:

$$R + T = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 |A|^2 \frac{k_1 \hbar}{m} + \frac{4k_1^2}{(k_1 + k_2)^2} |A|^2 \frac{k_2 \hbar}{m}, \tag{4.24}$$

$$\therefore R + T = |A|^2 \frac{k_1 \hbar}{m} \frac{k_1^2 - 2k_1 k_2 + k_2^2 + 4k_1 k_2}{(k_1 + k_2)^2}, \tag{4.25}$$

$$\therefore R + T = I. \tag{4.26}$$

In summary, a beam of particles each of which has energy E, incident on a potential step (cf. Fig. IV. 4.1) of height V_0, $E > V_0$, is partially reflected and partially transmitted. This should be compared with the classical situation where all the beam would be transmitted. Further, the conserved quantity is the flux (eq. (4.20)).

$\boxed{\text{CASE II : } E < V_0}$

Equation (4.1) can be written in the form of eq. (2.3), but eq. (4.2) takes the form

$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2}(V_0 - E)\psi(x) = k_2^2\psi(x), \qquad (4.27)$$

where

$$k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \text{ (real and positive).} \qquad (4.28)$$

Thus, the solutions for $\psi(x)$ are, for region I

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}, \qquad (4.29)$$

and for region II

$$\psi_{II}(x) = Ce^{k_2x} + De^{-k_2x}. \qquad (4.30)$$

The exponentials in eq. (4.30) are real, not complex. We require that $\psi_{II}(x)$ remain finite for $x \to +\infty$. Hence, we must have

$$C = 0, \qquad (4.31)$$

where it should be noted that we have taken the positive root for k_2 in eq. (4.28).

The solutions to the Schrödinger equation for regions I and II are (again) required to obey the continuity conditions at $x=0$. Thus,

$$A + B = D \qquad (4.32)$$

and

$$i k_1 (A - B) = -k_2 D, \qquad (4.33)$$

or

$$A - B = i \frac{k_2}{k_1} D. \qquad (4.34)$$

Adding eqs. (4.32) and (4.34),

$$2A = \left(1 + i\frac{k_2}{k_1}\right) D,$$

whence

$$\frac{D}{A} = \frac{2}{(1 + i k_2/k_1)} ; \qquad (4.35)$$

and subtracting eq. (4.34) from eq. (4.32),

$$2B = \left(1 - i\frac{k_2}{k_1}\right) D, \qquad (4.36)$$

whence from eq. (4.35)

$$\frac{B}{A} = \frac{(1 - i k_2/k_1)}{(1 + i k_2/k_1)}. \qquad (4.37)$$

It follows directly that (cf. eqs. (4.21) and (4.22))

$$\frac{R}{I} = \frac{|B|^2}{|A|^2} = \cancel{\frac{(1 - i k_2/k_1)}{(1 + i k_2/k_1)}}\,\cancel{\frac{(1 + i k_2/k_1)}{(1 - i k_2/k_1)}} = 1, \qquad (4.38)$$

i.e. the beam is <u>totally reflected</u>, as would be expected from the classical situation.

Although for $E < V_0$ the beam is totally reflected, the solution to the Schrödinger equation in region II is

$$\psi_{II}(x) = D e^{-k_2 x}, \tag{4.39}$$

i.e. a decaying exponential. In other words, the beam penetrates the barrier but is completely expelled back towards the source. From eq. (4.38) we must conclude that there is no flux associated with region II. To discuss this we must derive a more sophisticated expression for flux than the one given in eq. (4.20). This leads to the definition of <u>probability current density</u> which is detailed in the box below.