Problem 2.53

The Scattering Matrix. The theory of scattering generalizes in a pretty obvious way to arbitrary localized potentials (Figure 2.21). To the left (Region I), $V(x) = 0$, so

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}. \tag{2.178}$$

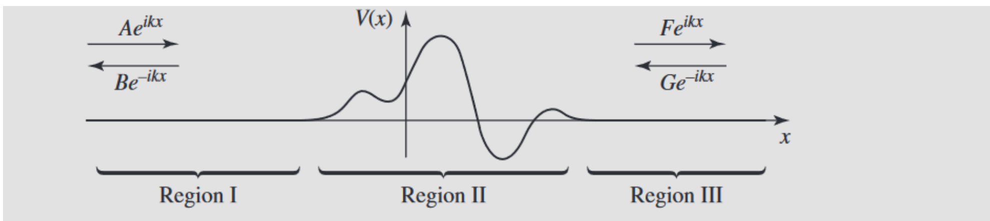

Figure 2.21: Scattering from an arbitrary localized potential ($V(x) = 0$ except in Region II); Problem 2.53.

To the right (Region III), $V(x)$ is again zero, so

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}. \tag{2.179}$$

In between (Region II), of course, I can't tell you what ψ is until you specify the potential, but because the Schrödinger equation is a linear, second-order differential equation, the general solution has got to be of the form

$$\psi(x) = Cf(x) + Dg(x),$$

where $f(x)$ and $g(x)$ are two linearly independent particular solutions.[63] There will be four boundary conditions (two joining Regions I and II, and two joining Regions II and III). Two of these can be used to eliminate C and D, and the other two can be "solved" for B and F in terms of A and G:

$$B = S_{11}A + S_{12}G, \quad F = S_{21}A + S_{22}G.$$

The four coefficients S_{ij}, which depend on k (and hence on E), constitute a 2×2 matrix $\mathbf{S}$, called the **scattering matrix** (or **S-matrix**, for short). The S-matrix tells you the outgoing amplitudes (B and F) in terms of the incoming amplitudes (A and G):

$$\begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix}. \tag{2.180}$$

In the typical case of scattering from the left, $G = 0$, so the reflection and transmission coefficients are

$$R_l = \left.\frac{|B|^2}{|A|^2}\right|_{G=0} = |S_{11}|^2, \quad T_l = \left.\frac{|F|^2}{|A|^2}\right|_{G=0} = |S_{21}|^2. \tag{2.181}$$

For scattering from the right, $A = 0$, and

$$R_r = \left.\frac{|F|^2}{|G|^2}\right|_{A=0} = |S_{22}|^2, \quad T_r = \left.\frac{|B|^2}{|G|^2}\right|_{A=0} = |S_{12}|^2. \tag{2.182}$$

[63] See any book on differential equations—for example, John L. Van Iwaarden, *Ordinary Differential Equations with Numerical Techniques*, Harcourt Brace Jovanovich, San Diego, 1985, Chapter 3.

(a) Construct the S-matrix for scattering from a delta-function well (Equation 2.117).

(b) Construct the S-matrix for the finite square well (Equation 2.148). *Hint:* This requires no new work, if you carefully exploit the symmetry of the problem.

Solution

Part (a)

With

$$V(x) = -\alpha\delta(x), \tag{2.117}$$

the Schrödinger equation becomes

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - \alpha\delta(x)\Psi(x,t), \quad -\infty < x < \infty,\ t > 0.$$

Applying the method of separation of variables $[\Psi(x,t) = \psi(x)\phi(t)]$ results in two ODEs, one in x and one in t.

$$\left.\begin{aligned} i\hbar\frac{\phi'(t)}{\phi(t)} &= E \\ -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} - \alpha\delta(x) &= E \end{aligned}\right\}$$

Solve the TISE for the second derivative.

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}[\alpha\delta(x) + E]\psi(x) \tag{1}$$

The delta function is zero everywhere except $x = 0$.

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x), \quad x \neq 0$$

For scattering states, $E > 0$, which means the general solution is

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x < 0 \\ Fe^{ikx} + Ge^{-ikx} & \text{if } x > 0 \end{cases},$$

where $k = \sqrt{2mE}/\hbar$. The wave function [and consequently $\psi(x)$] is required to be continuous at $x = 0$.

$$\lim_{x\to 0^-}\psi(x) = \lim_{x\to 0^+}\psi(x): \quad A + B = F + G \tag{2}$$

Integrate both sides of equation (1) with respect to x from $-\epsilon$ to ϵ, where ϵ is a really small positive number.

$$\begin{aligned} \int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}\,dx &= -\frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon}[\alpha\delta(x) + E]\psi(x)\,dx \\ \left.\frac{d\psi}{dx}\right|_{-\epsilon}^{\epsilon} &= -\frac{2m}{\hbar^2}\left[\alpha\int_{-\epsilon}^{\epsilon}\delta(x)\psi(x)\,dx + E\int_{-\epsilon}^{\epsilon}\psi(x)\,dx\right] \\ &= -\frac{2m}{\hbar^2}\left[\alpha\psi(0) + E\psi(0)\int_{-\epsilon}^{\epsilon}dx\right] \\ &= -\frac{2m}{\hbar^2}\left[\alpha\psi(0) + E\psi(0)(2\epsilon)\right] \end{aligned}$$

Take the limit as $\epsilon \to 0$.

$$\left.\frac{d\psi}{dx}\right|_{0^-}^{0^+} = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

The spatial derivative of the wave function, on the other hand, is discontinuous at $x = 0$.

$$\lim_{x\to 0^+}\frac{d\psi}{dx} - \lim_{x\to 0^-}\frac{d\psi}{dx} = -\frac{2m\alpha}{\hbar^2}\psi(0): \quad ik(F-G) - ik(A-B) = -\frac{2m\alpha}{\hbar^2}(A+B) \tag{3}$$

Solve equations (2) and (3) for B and F.

$$B = \frac{im\alpha}{k\hbar^2 - im\alpha}A + \frac{k\hbar^2}{k\hbar^2 - im\alpha}G = S_{11}A + S_{12}G$$

$$F = \frac{k\hbar^2}{k\hbar^2 - im\alpha}A + \frac{im\alpha}{k\hbar^2 - im\alpha}G = S_{21}A + S_{22}G$$

Therefore, the scattering matrix for the delta-function well is

$$\mathsf{S} = \begin{pmatrix} \frac{im\alpha}{k\hbar^2 - im\alpha} & \frac{k\hbar^2}{k\hbar^2 - im\alpha} \\ \frac{k\hbar^2}{k\hbar^2 - im\alpha} & \frac{im\alpha}{k\hbar^2 - im\alpha} \end{pmatrix}.$$

Part (b)

Now solve the Schrödinger equation,

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi(x,t), \quad -\infty < x < \infty,\ t > 0,$$

with

$$V(x) = \begin{cases} -V_0 & \text{if } -a \le x \le a \\ 0 & \text{if } |x| > a \end{cases}, \tag{2.148}$$

Applying the method of separation of variables $[\Psi(x,t) = \psi(x)\phi(t)]$ results in two ODEs, one in x and one in t.

$$\left.\begin{aligned} i\hbar\frac{\phi'(t)}{\phi(t)} &= E \\ -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x) &= E \end{aligned}\right\}$$

Solve the TISE for the second derivative.

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[V(x) - E]\psi(x) \tag{4}$$

For scattering states, $E > 0$, which means the general solution is

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x < -a \\ C\sin(lx) + D\cos(lx) & \text{if } -a \le x \le a \\ Fe^{ikx} + Ge^{-ikx} & \text{if } x > a \end{cases},$$

where

$$k = \frac{\sqrt{2mE}}{\hbar} \quad \text{and} \quad l = \frac{\sqrt{2m(V_0 + E)}}{\hbar}.$$

Require the wave function [and consequently $\psi(x)$] to be continuous at $x = -a$.

$$\lim_{x \to -a^-} \psi(x) = \lim_{x \to -a^+} \psi(x) : \quad Ae^{-ika} + Be^{ika} = -C \sin(la) + D \cos(la) \tag{5}$$

Require the wave function to be continuous at $x = a$ as well.

$$\lim_{x \to a^-} \psi(x) = \lim_{x \to a^+} \psi(x) : \quad C \sin(la) + D \cos(la) = Fe^{ika} + Ge^{-ika} \tag{6}$$

Integrate both sides of equation (4) with respect to x from $-a - \epsilon$ to $-a + \epsilon$, where ϵ is a really small positive number.

$$\begin{aligned} \int_{-a-\epsilon}^{-a+\epsilon} \frac{d^2\psi}{dx^2}\, dx &= \frac{2m}{\hbar^2} \int_{-a-\epsilon}^{-a+\epsilon} [V(x) - E]\psi(x)\, dx \\ \left.\frac{d\psi}{dx}\right|_{-a-\epsilon}^{-a+\epsilon} &= \frac{2m}{\hbar^2} \left[\int_{-a-\epsilon}^{-a} (0 - E)\, dx + \int_{-a}^{-a+\epsilon} (-V_0 - E)\, dx \right] \\ &= \frac{2m}{\hbar^2} [(-E)(\epsilon) + (-V_0 - E)(\epsilon)] \end{aligned}$$

Take the limit as $\epsilon \to 0$.

$$\left.\frac{d\psi}{dx}\right|_{-a^-}^{-a^+} = 0$$

It turns out that the spatial derivative of the wave function $\partial\Psi/\partial x$ is continuous at $x = -a$.

$$\lim_{x \to -a^-} \frac{d\psi}{dx} = \lim_{x \to -a^+} \frac{d\psi}{dx} : \quad ik(Ae^{-ika} - Be^{ika}) = l[C \cos(la) + D \sin(la)] \tag{7}$$

Now integrate both sides of equation (4) with respect to x from $a - \epsilon$ to $a + \epsilon$.

$$\begin{aligned} \int_{a-\epsilon}^{a+\epsilon} \frac{d^2\psi}{dx^2}\, dx &= \frac{2m}{\hbar^2} \int_{a-\epsilon}^{a+\epsilon} [V(x) - E]\psi(x)\, dx \\ \left.\frac{d\psi}{dx}\right|_{a-\epsilon}^{a+\epsilon} &= \frac{2m}{\hbar^2} \left[\int_{a-\epsilon}^{a} (-V_0 - E)\, dx + \int_{a}^{a+\epsilon} (0 - E)\, dx \right] \\ &= \frac{2m}{\hbar^2} [(-V_0 - E)(\epsilon) + (-E)(\epsilon)] \end{aligned}$$

Take the limit as $\epsilon \to 0$.

$$\left.\frac{d\psi}{dx}\right|_{a^-}^{a^+} = 0$$

It turns out that the spatial derivative of the wave function $\partial\Psi/\partial x$ is also continuous at $x = a$.

$$\lim_{x \to a^-} \frac{d\psi}{dx} = \lim_{x \to a^+} \frac{d\psi}{dx} : \quad l[C \cos(la) - D \sin(la)] = ik(Fe^{ika} - Ge^{-ika}) \tag{8}$$

To summarize, there are four equations involving A, B, C, D, E, and F.

$$\begin{cases} Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la) \\ C\sin(la) + D\cos(la) = Fe^{ika} + Ge^{-ika} \\ ik(Ae^{-ika} - Be^{ika}) = l[C\cos(la) + D\sin(la)] \\ l[C\cos(la) - D\sin(la)] = ik(Fe^{ika} - Ge^{-ika}) \end{cases}$$

Solve for B and F, eliminating C and D.

$$B = \frac{i(l^2 - k^2)e^{-2ika}\sin 2la}{2lk\cos 2la - i(l^2 + k^2)\sin 2la}A + \frac{2lke^{-2ika}}{2lk\cos 2la - i(l^2 + k^2)\sin 2la}G$$

$$F = \frac{2lke^{-2ika}}{2lk\cos 2la - i(l^2 + k^2)\sin 2la}A + \frac{i(l^2 - k^2)e^{-2ika}\sin 2la}{2lk\cos 2la - i(l^2 + k^2)\sin 2la}G$$

Therefore, the scattering matrix for the finite square well is

$$\mathsf{S} = \begin{pmatrix} \dfrac{i(l^2 - k^2)e^{-2ika}\sin 2la}{2lk\cos 2la - i(l^2 + k^2)\sin 2la} & \dfrac{2lke^{-2ika}}{2lk\cos 2la - i(l^2 + k^2)\sin 2la} \\ \dfrac{2lke^{-2ika}}{2lk\cos 2la - i(l^2 + k^2)\sin 2la} & \dfrac{i(l^2 - k^2)e^{-2ika}\sin 2la}{2lk\cos 2la - i(l^2 + k^2)\sin 2la} \end{pmatrix}.$$