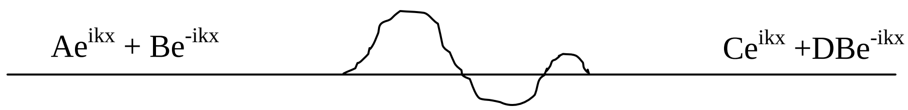
Gasiorowicz 3rd edition Feb 26, 2008

P4-1.

Consider an arbitrary potential localized on a finite part of the x-axis. The solutions os the Schrödinger equation to the left and to the right of the potential region are given by



respectively. Show that if we write

$$C = S_{11}A + S_{12}D$$
$$B = S_{21}A + S_{22}D$$

that is, relate the “outgoing” waves to the “ingoing” waves by

$$\begin{pmatrix} C \\ B \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix}$$

then the following relations hold

$$|S_{11}|^2 + |S_{21}|^2 = 1$$
$$|S_{12}|^2 + |S_{22}|^2 = 1$$
$$S_{11}S_{12}^* + S_{21}S_{22}^* = 0$$

Use this to show that the matrix

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

and its transpose are unitary. (Hint: Use flux conservation and the possibility that A and D are arbitrary complex numbers.)

Solution:

If $C = S_{11}A + S_{12}D$

$B = S_{21}A + S_{22}D$

$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$

$$\therefore\ j_I = \frac{\hbar k}{m}(|A|^2 - |B|^2)$$

$$= \frac{\hbar k}{m}[A^*A - (S_{21}^*A^* + S_{22}^*D^*)(S_{21}A + S_{22}D)]$$

$$= \frac{\hbar k}{m}[A^*A - (S_{21}^*S_{21}A^*A + S_{21}^*S_{22}A^*D + S_{21}S_{22}^*AD^* + S_{22}^*S_{22}D^*D)]$$

$\psi_{II}(x) = Ce^{ikx} + De^{-ikx}$

$$\therefore\ j_{II} = \frac{\hbar k}{m}(|C|^2 - |D|^2)$$

$$= \frac{\hbar k}{m}[(S_{11}^*A^* + S_{12}^*D^*)(S_{11}A + S_{12}D) - D^*D]$$

$$= \frac{\hbar k}{m}[(S_{11}^*S_{11}AA^* + S_{11}^*A^*S_{12}D + S_{12}^*S_{11}AD^* + S_{12}^*S_{12}DD^*) - D^*D]$$

Flux conservation $j_I = j_{II}$

$$\Rightarrow \frac{\hbar k}{m}[A^*A - (S_{21}^*S_{21}A^*A + S_{21}^*S_{22}A^*D + S_{21}S_{22}^*AD^* + S_{22}^*S_{22}D^*D)]$$

$$= \frac{\hbar k}{m}[(S_{11}^*S_{11}AA^* + S_{11}^*S_{12}A^*D + S_{12}^*S_{11}AD^* + S_{12}^*S_{12}DD^*) - D^*D]$$

$$\Rightarrow (1 - S_{21}^*S_{21} - S_{11}^*S_{11})AA^* - (S_{21}^*S_{22} + S_{11}^*S_{12})A^*D - (S_{21}S_{22}^* + S_{12}^*S_{11})AD^*$$
$$+ (1 - S_{22}^*S_{22} - S_{12}^*S_{12})D^*D = 0$$

Since A and D are arbitrary complex numbers, we require all coefficients of AA^*, A^*D, AD^* and D^*D to be zero :

Coefficient of $A^*A = 0$:

$$1 - S_{21}^*S_{21} - S_{11}^*S_{11} = 0 \Rightarrow S_{11}^*S_{11} + S_{21}^*S_{21} = 1 \Rightarrow |S_{11}|^2 + |S_{21}|^2 = 1$$

Coefficient of $A^*D = 0$:

$$S_{21}^*S_{22} + S_{11}^*S_{12} = 0 \Rightarrow (S_{21}^*S_{22} + S_{11}^*S_{12})^* = 0 \Rightarrow S_{11}S_{12}^* + S_{21}S_{22}^* = 0$$

Coefficient of $AD^* = 0$:

$$S_{21}S_{22}^* + S_{12}^*S_{11} = 0 \Rightarrow S_{11}S_{12}^* + S_{21}S_{22}^* = 0 \quad \text{(same as the last condition)}$$

Coefficient of $DD^* = 0$:

$$1 - S_{22}^*S_{22} - S_{12}^*S_{12} = 0 \Rightarrow S_{12}^*S_{12} + S_{22}^*S_{22} = 1 \Rightarrow |S_{12}|^2 + |S_{22}|^2 = 1$$

In summary,

$$S_{11}^*S_{11} + S_{21}^*S_{21} = 1$$

$$S_{11}S_{12}^* + S_{21}S_{22}^* = 0 \text{ or } S_{11}^*S_{12} + S_{21}^*S_{22} = 0$$

$$S_{12}^*S_{12} + S_{22}^*S_{22} = 1$$

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

$$S^+ = \begin{pmatrix} S_{11}^* & S_{21}^* \\ S_{12}^* & S_{22}^* \end{pmatrix}$$

$$S^+S = \begin{pmatrix} S_{11}^* & S_{21}^* \\ S_{12}^* & S_{22}^* \end{pmatrix}\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} S_{11}^*S_{11} + S_{21}^*S_{21} & S_{11}^*S_{12} + S_{21}^*S_{22} \\ S_{12}^*S_{11} + S_{22}^*S_{21} & S_{12}^*S_{12} + S_{22}^*S_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

This is enough to ensure $SS^+ = I$ also. If you want to calculate SS^+ explicitly:

$$S_{11}^*S_{11} + S_{21}^*S_{21} = 1 \qquad \text{---}(1)$$

$$S_{11}S_{12}^* + S_{21}S_{22}^* = 0 \text{ or } S_{11}^*S_{12} + S_{21}^*S_{22} = 0 \qquad \text{---}(2)$$

$$S_{12}^*S_{12} + S_{22}^*S_{22} = 1 \qquad \text{---}(3)$$

$$(2) \Rightarrow S_{21} = -\frac{S_{11}}{S_{22}^*}S_{12}^* \text{ and } S_{21}^* = -\frac{S_{11}^*}{S_{22}}S_{12}$$

$$\therefore S_{21}S_{21}^* = \frac{S_{11}S_{11}^*}{S_{22}S_{22}^*}S_{12}S_{12}^* \quad \text{---}(*) \text{ or } S_{12}S_{12}^* = \frac{S_{22}S_{22}^*}{S_{11}S_{11}^*}S_{21}S_{21}^* \quad \text{---}(**)$$

Substitute (*) into (1):

$$S_{11}^*S_{11} + \frac{S_{11}S_{11}^*}{S_{22}S_{22}^*}S_{12}S_{12}^* = 1 \Rightarrow S_{11}^*S_{11} + \frac{S_{11}S_{11}^*}{1 - S_{12}S_{12}^*}S_{12}S_{12}^* = 1 \quad (S_{22}S_{22}^* = 1 - S_{12}S_{12}^* \text{ from (3)})$$

$$\Rightarrow S_{11}^*S_{11} = 1 - S_{12}S_{12}^*$$

$$\Rightarrow \underline{S_{11}^*S_{11} + S_{12}S_{12}^* = 1}$$

Similarly substitute (**) into (3):

$$\frac{S_{22}S_{22}^*}{S_{11}S_{11}^*}S_{21}S_{21}^* + S_{22}^*S_{22} = 1 \Rightarrow \frac{S_{22}S_{22}^*}{1 - S_{21}^*S_{21}}S_{21}S_{21}^* + S_{22}^*S_{22} = 1 \quad (S_{11}^*S_{11} = 1 - S_{21}^*S_{21} \text{ from (1)})$$

$$\Rightarrow S_{22}^*S_{22} = 1 - S_{21}^*S_{21}$$

$$\Rightarrow \underline{S_{22}^*S_{22} + S_{21}^*S_{21} = 1}$$

But $(3) \Rightarrow S_{12}^*S_{12} + S_{22}^*S_{22} = 1$

$$\therefore S_{12}^*S_{12} + S_{22}^*S_{22} = S_{22}^*S_{22} + S_{21}^*S_{21} = 1 \Rightarrow S_{12}^*S_{12} = S_{21}^*S_{21} \Rightarrow S_{21}^* = \frac{S_{12}^*S_{12}}{S_{21}}$$

Substitute this into (2):

$$S_{11}^*S_{12} + S_{21}^*S_{22} = 0 \Rightarrow S_{11}^*S_{12} + \frac{S_{12}^*S_{12}}{S_{21}}S_{22} = 0 \Rightarrow \underline{S_{11}^*S_{21} + S_{12}^*S_{22} = 0 \text{ or } S_{21}^*S_{11} + S_{22}^*S_{12} = 0}$$

In summary,

$$S_{11}^*S_{11} + S_{12}S_{12}^* = 1$$

$$S_{22}^*S_{22} + S_{21}^*S_{21} = 1$$

$$S_{11}^*S_{21} + S_{12}^*S_{22} = 0 \text{ or } S_{21}^*S_{11} + S_{22}^*S_{12} = 0$$

Now we can calculate

$$S\,S^+ = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}\begin{pmatrix} S_{11}^* & S_{21}^* \\ S_{12}^* & S_{22}^* \end{pmatrix} = \begin{pmatrix} S_{11}S_{11}^* + S_{12}S_{12}^* & S_{11}S_{21}^* + S_{12}S_{22}^* \\ S_{21}S_{11}^* + S_{22}S_{12}^* & S_{21}S_{21}^* + S_{22}S_{22}^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$\therefore S^+S = S\,S^+ = I$, S is unitary.

For transpose, let $T = S^T$

$$\therefore T = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}^T = \begin{pmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{pmatrix}$$

$$T^+ = \begin{pmatrix} S_{11}^* & S_{12}^* \\ S_{21}^* & S_{22}^* \end{pmatrix}$$

$$TT^+ = \begin{pmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{pmatrix}\begin{pmatrix} S_{11}^* & S_{12}^* \\ S_{21}^* & S_{22}^* \end{pmatrix} = \begin{pmatrix} S_{11}S_{11}^* + S_{21}S_{21}^* & S_{11}S_{12}^* + S_{21}S_{22}^* \\ S_{12}S_{11}^* + S_{22}S_{21}^* & S_{12}S_{12}^* + S_{22}S_{22}^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Similarly,

$$T^+T = \begin{pmatrix} S_{11}^* & S_{12}^* \\ S_{21}^* & S_{22}^* \end{pmatrix}\begin{pmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{pmatrix} = \begin{pmatrix} S_{11}^*S_{11} + S_{12}^*S_{12} & S_{11}^*S_{21} + S_{12}^*S_{22} \\ S_{21}^*S_{11} + S_{22}^*S_{12} & S_{21}^*S_{21} + S_{22}^*S_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

So T (transpose of S) is also unitary.