TRANSFER MATRIX

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.53.

We've seen that in the general scattering problem, we can write the particle stream magnitudes on each side of the potential by using a scattering matrix. In general, the wave function in the left hand region where $V=0$ is

$$\psi_l = Ae^{ikx} + Be^{-ikx} \tag{1}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \tag{2}$$

On the right,

$$\psi_r = Fe^{ikx} + Ge^{-ikx} \tag{3}$$

We can relate the coefficients by using the matrix

$$\begin{bmatrix} B \\ F \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} A \\ G \end{bmatrix} \tag{4}$$

This expresses the outgoing particle streams on each side in terms of the incoming streams.

We can also express the streams on the right in terms of the streams on the left by using a *transfer matrix*. That is, we can write

$$\begin{bmatrix} F \\ G \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} \tag{5}$$

By solving the scattering matrix equation for F and G in terms of A and B we can express the transfer matrix in terms of the scattering matrix.

$$\mathsf{M} = -\frac{1}{S_{12}} \begin{bmatrix} S_{11}S_{22} - S_{12}S_{21} & -S_{22} \\ S_{11} & -1 \end{bmatrix} \tag{6}$$

The element M_{11} is just the determinant of S so we have

$$\mathsf{M}=-\frac{1}{S_{12}}\begin{bmatrix}\det\mathsf{S} & -S_{22}\\ S_{11} & -1\end{bmatrix} \tag{7}$$

Conversely, we can express the scattering matrix in terms of the transfer matrix:

$$\mathsf{S}=\frac{1}{M_{22}}\begin{bmatrix}-M_{21} & 1\\ \det\mathsf{M} & M_{12}\end{bmatrix} \tag{8}$$

In the special case where the only incoming particles are from the left, $G=0$ and from the scattering matrix, we have for the reflection coefficient

$$R_l = \frac{|B|^2}{|A|^2} \tag{9}$$
$$= |S_{11}|^2 \tag{10}$$
$$= \frac{|M_{21}|^2}{|M_{22}|^2} \tag{11}$$

For the transmission coefficient

$$T_l = \frac{|F|^2}{|A|^2} \tag{12}$$
$$= |S_{21}|^2 \tag{13}$$
$$= \frac{|\det\mathsf{M}|^2}{|M_{22}|^2} \tag{14}$$

If the incoming particles are from the right only, $A=0$ and we get

$$R_r = \frac{|F|^2}{|G|^2} \tag{15}$$
$$= |S_{22}|^2 \tag{16}$$
$$= \frac{|M_{12}|^2}{|M_{22}|^2} \tag{17}$$

$$T_r = \frac{|B|^2}{|G|^2} \tag{18}$$

$$= |S_{12}|^2 \tag{19}$$

$$= \frac{1}{|M_{22}|^2} \tag{20}$$

Now suppose we have a potential which is non-zero in only two isolated regions. For example, we could have two finite square wells separated by a gap, or a double delta function well. To the left of the leftmost non-zero region, the wave function is

$$\psi_1 = Ae^{ikx} + Be^{-ikx} \tag{21}$$

In between the two regions, we have

$$\psi_2 = Ce^{ikx} + De^{-ikx} \tag{22}$$

and to the right of the second region we have

$$\psi_3 = Fe^{ikx} + Ge^{-ikx} \tag{23}$$

We cannot say what the wave function within either region is unless we specify the potential there, of course.

In terms of the transfer matrix, the transition from region 1 to region 2 is given by

$$\begin{bmatrix} C \\ D \end{bmatrix} = \mathsf{M}_1 \begin{bmatrix} A \\ B \end{bmatrix} \tag{24}$$

Between regions 2 and 3, we have

$$\begin{bmatrix} F \\ G \end{bmatrix} = \mathsf{M}_2 \begin{bmatrix} C \\ D \end{bmatrix} = \mathsf{M}_2\mathsf{M}_1 \begin{bmatrix} A \\ B \end{bmatrix} \tag{25}$$

Thus the overall transfer matrix is the product of the two individual ones:

$$\mathsf{M} = \mathsf{M}_2\mathsf{M}_1 \tag{26}$$

This result generalizes to any potential that consists of a number of distinct regions where it is non-zero.

As an example, we can consider the delta function well again, except this time we'll position the well at some arbitrary location $x = a$, so we have

$$V(x) = -\alpha\delta(x-a) \tag{27}$$

In this case, we have two regions, so we can write

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < a \\ Fe^{ikx} + Ge^{-ikx} & x > a \end{cases} \tag{28}$$

Following the same analysis as in the original delta function at the origin, we have a couple of boundary conditions at $x = a$. From continuity of the wave function we have

$$Ae^{ika} + Be^{-ika} = Fe^{ika} + Ge^{-ika} \tag{29}$$

The first derivative is discontinuous, and we get the condition

$$\Delta\psi' = -\frac{2m\alpha}{\hbar^2}\psi(a) \tag{30}$$

$$ik\left[(F-A)e^{ika} - (G-B)e^{-ika}\right] = -\frac{2m\alpha}{\hbar^2}\left[Ae^{ika} + Be^{-ika}\right] \tag{31}$$

Solving these two equations in terms of A and B we can read off the transfer matrix

$$\mathsf{M} = \frac{1}{2k}\left[\begin{array}{cc} 2k + iz & ize^{-2ika} \\ ize^{2ika} & -2k + iz \end{array}\right] \tag{32}$$

where

$$z \equiv \frac{2m\alpha}{\hbar^2} \tag{33}$$

We can now reconsider the double delta well problem by applying the product of transfer matrixes above. The potential is

$$V(x) = -\alpha\left[\delta(x+a) + \delta(x-a)\right] \tag{34}$$

We already have the transfer matrix for the $\delta(x-a)$ part of the potential, which we'll call M_2 since it's on the right hand side. We can get the other transfer matrix by substituting $-a$ for a:

$$\mathsf{M}_2 = \frac{1}{2k}\begin{bmatrix} 2k+iz & ize^{2ika} \\ ize^{-2ika} & -2k+iz \end{bmatrix} \tag{35}$$

The transfer matrix for the combined potential is then $\mathsf{M} = \mathsf{M}_2\mathsf{M}_1$ so we get

(36)
$$\mathsf{M} = \frac{1}{4k^2}\begin{bmatrix} z^2\left(e^{-4ika}-1\right)+4k^2+4ikz & i\left[4k\cos(2ka)-2z\sin(2ka)\right] \\ -i\left[4k\cos(2ka)-2z\sin(2ka)\right] & z^2\left(e^{4ika}-1\right)+4k^2-4ikz \end{bmatrix}$$

As a check, we can work out the transmission coefficient for the case $G=0$ and compare it with our earlier result. From above, we have

$$T_l = \frac{|\det \mathsf{M}|^2}{|M_{22}|^2} \tag{37}$$

The determinant conveniently works out to

$$\det \mathsf{M} = 1 \tag{38}$$

so we get

$$T_l = \frac{8k^4}{8k^4+4k^2z^2+z^4-4kz^3\sin(4ka)+z^2\cos(4ka)\left[4k^2-z^2\right]} \tag{39}$$

which is the same as the result we got previously.