Appendix A4

A4.1 BOUNDARY MATRICES

In this appendix we present another matrix method for calculating reflection from complex surfaces. This method has more complicated matrix elements but a simpler relation between the matrix elements and the reflection and transmission amplitudes than those of section 2.4.4. These matrices are based on relations between the coefficients of the two linearly independent solutions within a given layer. We assume the particles are incident from the left of the surface and number the layers with numbers increasing to the right.

Writing the wavefunction in the nth layer as (2.77) with coefficients A_n, B_n and denoting the wavevector in the region between (z_n, z_{n+1}) as k_n and that in the region (z_{n-1}, z_n) as k_{n-1}, we have as the boundary conditions at z_n

$$A_{n-1}\mathrm{e}^{\mathrm{i}k_{n-1}z_n} + B_{n-1}\mathrm{e}^{-\mathrm{i}k_{n-1}z_n} = A_n\mathrm{e}^{\mathrm{i}k_n z_n} + B_n\mathrm{e}^{-\mathrm{i}k_n z_n} \quad \text{(A4.1)}$$

$$k_{n-1}\left(A_{n-1}\mathrm{e}^{\mathrm{i}k_{n-1}z_n} - B_{n-1}\mathrm{e}^{-\mathrm{i}k_{n-1}z_n}\right) = k_n\left(A_n\mathrm{e}^{\mathrm{i}k_n z_n} - B_n\mathrm{e}^{-\mathrm{i}k_n z_n}\right) \quad \text{(A4.2)}$$

or solving for A_n and B_n we find

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \frac{1}{2}\begin{bmatrix} (1+\gamma_n)\,\mathrm{e}^{\mathrm{i}(k_{n-1}-k_n)z_n} & (1-\gamma_n)\,\mathrm{e}^{-\mathrm{i}(k_{n-1}+k_n)z_n} \\ (1-\gamma_n)\,\mathrm{e}^{\mathrm{i}(k_{n-1}+k_n)z_n} & (1+\gamma_n)\,\mathrm{e}^{-\mathrm{i}(k_{n-1}-k_n)z_n} \end{bmatrix} \cdot \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} \quad \text{(A4.3)}$$

$$\equiv \tilde{M}_n \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix}$$

with $\gamma_n = k_{n-1}/k_n$. Taking (2.48) for the wavefunction we have

$$\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = \begin{pmatrix} 1 \\ R \end{pmatrix} \quad \text{(A4.4)}$$

and taking (2.49) for the wavefunction inside the material, we have

$$\begin{pmatrix} T \\ 0 \end{pmatrix} = \bar{M} \begin{pmatrix} 1 \\ R \end{pmatrix} \tag{A4.5}$$

with

$$\bar{M} = \bar{M}_N \ldots \bar{M}_2 \cdot \bar{M}_1 = \begin{pmatrix} \bar{M}_{11} & \bar{M}_{12} \\ \bar{M}_{21} & \bar{M}_{22} \end{pmatrix}. \tag{A4.6}$$

From (A4.3) we have

$$\det\ \bar{M}_n = \gamma_n \tag{A4.7}$$

so that

$$\det\ \bar{M} = \frac{k_1}{k_2} \tag{A4.8}$$

and

$$R = \frac{-\bar{M}_{21}}{\bar{M}_{22}} \qquad T = \frac{k_1/k_2}{\bar{M}_{22}}. \tag{A4.9}$$

It is interesting to note that we can obtain the solution for particles travelling through the same barrier in the opposite direction by replacing (A4.5) by

$$\begin{pmatrix} \tilde{R} \\ 1 \end{pmatrix} = \bar{M} \cdot \begin{pmatrix} 0 \\ \tilde{T} \end{pmatrix} \tag{A4.10}$$

where $\tilde{T}$ and $\tilde{R}$ are the transmission and reflection amplitudes for this opposite direction (particles incident from the right) and $\bar{M}$ is the same as in (A4.6).

Thus we find

$$\tilde{T} = \frac{1}{\bar{M}_{22}} \qquad \tilde{R} = \frac{\bar{M}_{12}}{\bar{M}_{22}}. \tag{A4.11}$$

Thus

$$\frac{T}{\tilde{T}} = \frac{k_1}{k_2} \qquad \frac{R}{\tilde{R}} = \frac{-\bar{M}_{21}}{\bar{M}_{12}} \tag{A4.12}$$

for any barrier. Note that the matrices based on the linearly independent solutions (A4.3) each represent a single boundary while the matrices based on $\psi(x)$ and $\psi'(x)$ of section 2.4.4 each represent an entire layer.