Short notes on Matching wavefunctions in one dimension using transfer-matrices

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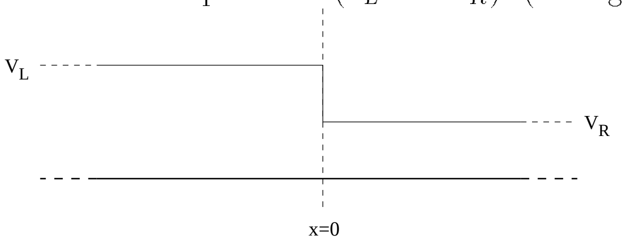
These notes are a short introduction in how to calculate the quantum-mechanical wavefunction in a one-dimensional, steplike potential, using transfer-matrices.

1 Transfer matrix for a single interface

Consider a one-dimensional potential consisting of two semi-infinite parts with constant potential (V_L and V_R). (See figure.)



We know that the eigenfunctions to the (time-independent) Schrödinger-equation in a constant potential (V) are the following:

$$\Psi_k(x) = A \cdot e^{\pm ikx} \tag{1}$$

$$E_k = V + \frac{\hbar^2 k^2}{2m} \tag{2}$$

$$V < E \Rightarrow k = \frac{1}{\hbar}\sqrt{2m(E-V)} \tag{3}$$

$$V > E \Rightarrow k = i\kappa \qquad \kappa = \frac{1}{\hbar}\sqrt{2m(V-E)} \tag{4}$$

To each energy larger than the potential energy correspond two plane waves. One travelling to the right and one travelling to the left. To each energy smaller than the potential energy correspond two exponentially decaying/growing wavefunctions. The general energy-eigenfunction is a linear combination of the two possible for that specific energy.

$$\Psi_E(x) = A \cdot e^{ikx} + B \cdot e^{-ikx} \tag{5}$$

For $E < V$ this equals:

$$\Psi_E(x) = A \cdot e^{-\kappa x} + B \cdot e^{\kappa x} \tag{6}$$

Now we have the solutions in each region and can compose the total solution. Because of the different potentials in the two regions we have, for the same energy, different k:s in the different regions. From quantum-mechanics we know how to match the eigenfunctions at the interface to get the total energy-eigenfunctions for the potential. We should make sure that both the wavefunctions themselves and their first derivatives are continuous across the interface. This gives us two equations for each energy.

$$A_L e^{ik_L x} + B_L e^{-ik_L x} = A_R e^{ik_R x} + B_R e^{-ik_R x} \tag{7}$$

$$A_L ik_L e^{ik_L x} + B_L(-ik_L)e^{-ik_L x} = A_R ik_R e^{ik_R x} + B_R(-ik_R)e^{-ik_R x} \tag{8}$$

Now we have the basic equations and we can easily solve them. It is here the transfer-matrix technique starts. Suppose that we know the coefficients in the left region, (A_L and B_L) for a specific energy-eigenfunction. Then, by solving the two equations above, we can get the coefficients in the right region. One simple way to do this is to rewrite the two equations as one matrix equation:

$$M_{Lx} \begin{pmatrix} A_L \\ B_L \end{pmatrix} = M_{Rx} \begin{pmatrix} A_R \\ B_R \end{pmatrix} \tag{9}$$

$$M_{Lx} = \begin{pmatrix} 1 & 1 \\ ik_L & -ik_L \end{pmatrix} \cdot \begin{pmatrix} e^{ik_L x} & 0 \\ 0 & e^{-ik_L x} \end{pmatrix} \tag{10}$$

$$M_{Rx} = \begin{pmatrix} 1 & 1 \\ ik_R & -ik_R \end{pmatrix} \cdot \begin{pmatrix} e^{ik_R x} & 0 \\ 0 & e^{-ik_R x} \end{pmatrix} \tag{11}$$

Now it is easy to get the coefficients in the right region:

$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = M_{Rx}^{-1} M_{Lx} \begin{pmatrix} A_L \\ B_L \end{pmatrix} \equiv T_{RLx} \begin{pmatrix} A_L \\ B_L \end{pmatrix} \tag{12}$$

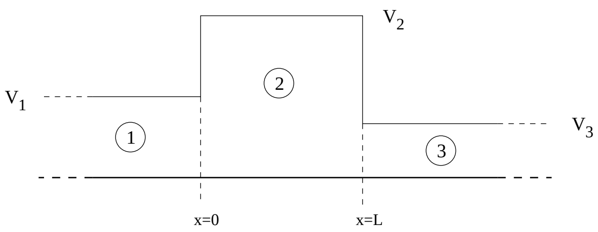
where we have defined the *transfer-matrix* $T_{RLx} \equiv M_{Rx}^{-1} M_{Lx}$. *So if we know coefficients to the left of the interface we can "transfer" them to the right of the interface just by multiplying with the transfer-matrix.*

$$\begin{aligned} T_{RLx} &= \begin{pmatrix} e^{-ik_R x} & 0 \\ 0 & e^{ik_R x} \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} 1 & \frac{1}{ik_R} \\ 1 & -\frac{1}{ik_R} \end{pmatrix} \cdot \begin{pmatrix} 1 & 1 \\ ik_L & -ik_L \end{pmatrix} \cdot \begin{pmatrix} e^{ik_L x} & 0 \\ 0 & e^{-ik_L x} \end{pmatrix} \\ &= \begin{pmatrix} e^{-ik_R x} & 0 \\ 0 & e^{ik_R x} \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} 1 + \frac{k_L}{k_R} & 1 - \frac{k_L}{k_R} \\ 1 - \frac{k_L}{k_R} & 1 + \frac{k_L}{k_R} \end{pmatrix} \cdot \begin{pmatrix} e^{ik_L x} & 0 \\ 0 & e^{-ik_L x} \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} (1 + \frac{k_L}{k_R}) e^{i(k_L - k_R)x} & (1 - \frac{k_L}{k_R}) e^{-i(k_L + k_R)x} \\ (1 - \frac{k_L}{k_R}) e^{i(k_L + k_R)x} & (1 + \frac{k_L}{k_R}) e^{-i(k_L - k_R)x} \end{pmatrix} \end{aligned} \tag{13}$$

For just one interface it maybe seems like overkill to rewrite the matching as a matrix-equation, but for more complex potentials the simplification will become apparent.

2 Transfer matrix for a barrier

Now consider the following potential with three different regions (labelled one, two and three). Regions one and three are semi-infinite while region two has the length L.



Now we want to establish the connection between the coefficients of an energy-eigenfunction in region three to its coefficients in region one. If we put the zero of the x-coordinate at the interface between region one and two we can use the technique above to get the coefficients in region two.

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = TM_{21(0)} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \tag{14}$$

To get the coefficients in region three we simply have to multiply the coefficients in region two by the correct transfer-matrix:

$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = TM_{32(L)} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = TM_{32(L)} \cdot TM_{21(0)} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \tag{15}$$

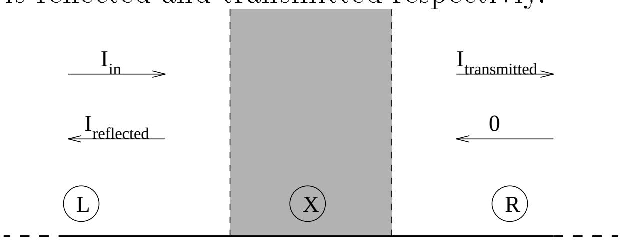
Now it is straightforward to define the total transfer-matrix by:

$$\begin{aligned} TM_{31} &= TM_{32(L)} \cdot TM_{21(0)} = \\ &= \begin{pmatrix} e^{-ik_3 L} & 0 \\ 0 & e^{ik_3 L} \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} 1+\frac{k_2}{k_3} & 1-\frac{k_2}{k_3} \\ 1-\frac{k_2}{k_3} & 1+\frac{k_2}{k_3} \end{pmatrix} \\ &\cdot \begin{pmatrix} e^{ik_2 L} & 0 \\ 0 & e^{-ik_2 L} \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} 1+\frac{k_1}{k_2} & 1-\frac{k_1}{k_2} \\ 1-\frac{k_1}{k_2} & 1+\frac{k_1}{k_2} \end{pmatrix} \end{aligned} \tag{16}$$

Both the name and the advantage of the transfer-matrices should now be clear. The transfer-matrices transfer the coefficients in one region to the coefficients in its neighbouring region by simple matrix multiplication. *Using just the above transfer-matrix one can treat any step-like potential structure.* The analytic form of the matrices may get quite complicated but that is no problem for a computer. *This method is very well suited for numerical studies.*

3 Reflection and transmision amplitudes

As an example of how to use the transfer matrices we can calculate the reflection- and transmission-amplitudes of any steplike structure. These amplitudes tell how much of a current that is incident on a structure that is reflected and transmitted respectivly.



$$R = \frac{I_{reflected}}{I_{in}} \tag{17}$$

$$D = \frac{I_{transmitted}}{I_{in}} \tag{18}$$

To calculate these quantities we first have to calculate the current from the energy-eigenfunctions. This is easy using the quantum-mechanical formula for current:

$$I = \frac{e\hbar}{2mi}(\Psi^* \nabla \Psi - (\nabla \Psi^*)\Psi) \tag{19}$$

Using this formula on the eigenfunctions gives the following result:

$$\begin{aligned} \Psi &= A \cdot e^{ikx} + B \cdot e^{-ikx} \\ k \quad real \quad (E > V) \;\Rightarrow\; I &= \frac{e\hbar k}{m}(|A|^2 - |B|^2) && (20) \\ k = i\kappa \quad (E < V) \;\Rightarrow\; I &= \frac{2e\hbar\kappa}{m} Im[AB^*] && (21) \end{aligned}$$

Using the transfer-matrix for the X-structure we have the following equation.

$$\begin{pmatrix} A_R \\ B_R \end{pmatrix} = TM_{RL} \begin{pmatrix} A_L \\ B_L \end{pmatrix} \tag{22}$$

Because we do not have any current incoming from the right we should put $B_R = 0$.

$$\begin{pmatrix} A_R \\ 0 \end{pmatrix} = TM_{RL} \begin{pmatrix} A_L \\ B_L \end{pmatrix} \tag{23}$$

Naming the matrix elements of the transfer-matrix t_{11}, t_{12}, t_{21} and t_{22} we get:

$$\begin{aligned} TM_{RL} &= \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} && (24) \\ B_L &= -\frac{t_{21}}{t_{22}} A_L && (25) \\ A_R &= \left(t_{11} - \frac{t_{12}t_{21}}{t_{22}}\right) A_L && (26) \\ R &= \frac{k_L |B_L|^2}{k_L |A_L|^2} = \left|\frac{t_{21}}{t_{22}}\right|^2 && (27) \\ D &= \frac{k_R |A_R|^2}{k_L |A_L|^2} = \frac{k_R}{k_L} \left|t_{11} - \frac{t_{12}t_{21}}{t_{22}}\right|^2 && (28) \end{aligned}$$

Due to current-conservation it is always true, in the time-independent case, that $R + D = 1$. This relation can be used to check that the transfer-matrix is correct.