Notes on the solution to 1D Schrdinger equation for piecewise potentials

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Brief rendition of the way to solve the Schrdinger equation for piecewise potentials

We consider the time independent 1D Schrdinger equation, (in natural units)

$$-\frac{1}{2}\partial_x^2\psi(x) + V(x)\psi(x) = E\psi(x)\,. \tag{1}$$

Where the potential is taken to be piecewise constant, that is,

$$V(x) = V_k \; x_k < x < x_{k+1}\,. \tag{2}$$

where $\{x_k\}$ is a partition of the interval $[0, L]$, and $k = 0, \ldots, N$. For simplicity we take the utmost left and right potentials to be infinite, that is, the wave function is zero at $x = 0$ and $x = L$. For each interval, $[x_k, x_{k+1}]$ the general solution of the Schrdinger equation reads,

$$\psi_k(x) = A_k e^{i\kappa_k x} + B_k e^{-i\kappa_k x} \tag{3}$$

where $\kappa_k = \sqrt{2(E - V_k)}$.

First we consider the first and last intervals,

$$\begin{aligned}\psi_0(x) &= A_0 e^{i\kappa_0 x} + B_0 e^{-i\kappa_0 x} \\ \psi_N(x) &= A_N e^{i\kappa_N x} + B_N e^{-i\kappa_N x}\end{aligned} \tag{4}$$

the boundary conditions imply,

$$\begin{aligned}\psi_0(x) &= A_0\left(e^{i\kappa_0 x} - e^{-i\kappa_0 x}\right) = A_0\, 2\, i\, \sin(\kappa_0 x) \\ \psi_N(x) &= A_N e^{i\kappa_N L}\left(e^{i\kappa_N(x-L)} - e^{-i\kappa_N(x-L)}\right) = A_N\, 2\, i\, \sin(\kappa_N(x-L))\end{aligned} \tag{5}$$

If we consider two inner intervals we have to impose continuity of the wave function and of its first derivative, that reads,

$$\begin{aligned}\psi_k(x_{k+1}) &= \psi_{k+1}(x_{k+1}) \\ \psi'_k(x_{k+1}) &= \psi'_{k+1}(x_{k+1})\end{aligned} \tag{6}$$

which read,

$$\begin{aligned}A_k e^{i\kappa_k x_{k+1}} + B_k e^{-i\kappa_k x_{k+1}} &= A_{k+1} e^{i\kappa_{k+1} x_{k+1}} + B_k e^{-i\kappa_{k+1} x_{k+1}} \\ A_k i\kappa_k e^{i\kappa_k x_{k+1}} - B_k i\kappa_k e^{-i\kappa_k x_{k+1}} &= A_{k+1} i\kappa_{k+1} e^{i\kappa_{k+1} x_{k+1}} - B_k i\kappa_{k+1} e^{-i\kappa_{k+1} x_{k+1}}\,.\end{aligned} \tag{7}$$

These can be written in matrix form as,

$$\begin{pmatrix} e^{i\kappa_k x_{k+1}} & e^{-i\kappa_k x_{k+1}} \\ i\kappa_k e^{i\kappa_k x_{k+1}} & -i\kappa_k e^{-i\kappa_k x_{k+1}} d\end{pmatrix}\begin{pmatrix}A_k \\ B_k\end{pmatrix} = \begin{pmatrix} e^{i\kappa_{k+1} x_{k+1}} & e^{-i\kappa_{k+1} x_{k+1}} \\ i\kappa_{k+1} e^{i\kappa_{k+1} x_{k+1}} & -i\kappa_{k+1} e^{-i\kappa_{k+1} x_{k+1}} d\end{pmatrix}\begin{pmatrix}A_{k+1} \\ B_{k+1}\end{pmatrix} \tag{8}$$

which can be written as,

$$\mathcal{M}(\kappa_k, x_{k+1})\phi_k = \mathcal{M}(\kappa_{k+1}, x_{k+1})\phi_{k+1} \tag{9}$$

where,

$$\mathcal{M}(\kappa, x) = \begin{pmatrix} e^{i\kappa x} & e^{-i\kappa x} \\ i\kappa e^{i\kappa x} & -i\kappa e^{-i\kappa x}\end{pmatrix} \qquad \phi_k = \begin{pmatrix}A_k \\ B_k\end{pmatrix} \tag{10}$$

This allows us to solve the wave function in the $k+1$ interval from the values in the k interval,

$$\phi_{k+1} = \mathcal{M}^{-1}(\kappa_{k+1}, x_{k+1})\mathcal{M}(\kappa_k, x_{k+1})\phi_k \tag{11}$$

where the inverse matrix reads,

$$\mathcal{M}^{-1}(\kappa, x) = \begin{pmatrix} \frac{1}{2}e^{-i\kappa x} & \frac{-i}{2\kappa}e^{-i\kappa x} \\ \frac{1}{2}e^{i\kappa x} & \frac{i}{2\kappa}e^{i\kappa x}\end{pmatrix} \tag{12}$$

A. how to find the eigenenergies?

To find the energy quantization we basicaly write the wave function in the last interval as a function of the wave function in the first interval,

$$\hat{\phi}_N = \mathcal{M}^{-1}(\kappa_N, x_N)\mathcal{M}(\kappa_{N-1}, x_N)\ldots\mathcal{M}^{-1}(\kappa_{j+1}, x_{j+1})\mathcal{M}(\kappa_j, x_{j+1})\ldots\mathcal{M}^{-1}(\kappa_1, x_1)\mathcal{M}(\kappa_0, x_1)\phi_0 \tag{13}$$

with $\phi_0 = \{A_0, -A_0\}$. This should indeed be equal to ϕ_N, that we wrote in Eq. (**??**).

Now for instance we do,

$$\hat{\phi}_N(1)/\hat{\phi}_N(2) - \phi_N(1)/\phi_N(2) = 0 \tag{14}$$

and look for values of E that solve the above equation. Notice in the above equation the values of A_0 and A_N.