Computing the eigen-energies of a 1D Schdinger equation for piecewise potentials

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Following BJD notes, for every piece of a piecewise potential

$$V(x) = \begin{cases} \infty & x < 0 \\ V_1 & 0 < x < x_1 \\ ... & ... \\ V_k & x_{k-1} < x < x_k \\ ... & ... \\ V_N & 0 < x < x_N \\ \infty & x > 1 \end{cases} \tag{1}$$

there will be a wave-function solution of the Schdinger equation

$$\psi(x) = \begin{cases} 0 & x < 0 \\ \psi_1 & 0 < x < x_1 \\ ... & ... \\ \psi_k & x_{k-1} < x < x_k \\ ... & ... \\ \psi_N & 0 < x < x_N \\ 0 & x > 1 \end{cases} \tag{2}$$

with the shape

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

and the wave number $\kappa_k = \sqrt{2(E - V_k)}$.

This piecewise wave will satisfy both a boundary condition at the infinite walls

$$\psi_1(x = 0) = \psi_N(x = 1) = 0 \tag{4}$$

and a continuity condition, for $k = 1...N - 1$,

$$\begin{aligned} \psi_k(x_k) &= \psi_{k+1}(x_k) \\ \psi'_k(x_k) &= \psi'_{k+1}(x_k). \end{aligned} \tag{5}$$

As suggested by BJD notes, we simplify the wave-function as

$$\psi_k(x) = A_k e^{i\kappa_k x} + B_k e^{-i\kappa_k x} \implies \phi_k = \begin{pmatrix} A_k \\ B_k \end{pmatrix} \tag{6}$$

and impose a boundary condition for the left wall

$$\psi_1(x = 0) = 0 \implies B_1 = -A_1 \implies \phi_1 = -A_1 \begin{pmatrix} 1 \\ -1 \end{pmatrix} \implies \tilde{\phi}_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{7}$$

We can work with the unnormalized form $\tilde{\phi}_0$ and leave the normalization of the whole wave for the end. Having $\tilde{\phi}_1$, we can find the others $\tilde{\phi}_k$ neighbour by neighbour with the continuity condition:

$$\left.\begin{aligned} \psi_k(x_k) = &\quad \psi_{k+1}(x_k) \\ \psi'_k(x_k) = &\quad \psi'_{k+1}(x_k) \end{aligned}\right\} \implies \mathcal{M}(\kappa_k, x_k)\tilde{\phi}_k = \mathcal{M}(\kappa_{k+1}, x_k)\tilde{\phi}_{k+1}$$

Which means that, in the simplified form, the continuity condition from $\tilde{\phi}_k$ to $\tilde{\phi}_{k+1}$ is a 2x2 matrix

$$\begin{aligned} \tilde{\phi}_2 &= \mathcal{M}^{-1}(\kappa_2, x_1)\mathcal{M}(\kappa_1, x_1)\tilde{\phi}_1 \\ \tilde{\phi}_3 &= \mathcal{M}^{-1}(\kappa_3, x_2)\mathcal{M}(\kappa_2, x_2)\tilde{\phi}_2 \\ &... \end{aligned} \tag{8}$$

Therefore, multiplying all the way from $\tilde{\phi}_1$ to $\tilde{\phi}_N$ we can compute

$$\begin{aligned} \tilde{\phi}_N &= \prod^{N-1} \mathcal{M}^{-1}\mathcal{M} \;\; \tilde{\phi}_1 \\ \begin{pmatrix} \tilde{A}_N \\ \tilde{B}_N \end{pmatrix} &= \qquad \mathcal{M}_{eff} \qquad \begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{aligned} \tag{9}$$

Here's the tricky part. Having imposed that the wave function is null on the left wall, only eigen-energies will null it on the right wall

$$\begin{array}{ccc} \psi_1(x) = A_1 e^{i\kappa_1 x} + B_1 e^{-i\kappa_1 x} & & \psi_N(x) = A_N e^{i\kappa_N x} + B_N e^{-i\kappa_N x} \\ \boxed{\psi_1(x=0) = 0} & \xrightarrow{if E=E_n} & \boxed{\psi_N(x=1) = 0} \\ \psi_1(x) = A_1 e^{i\kappa_1 x} + B_1 e^{-i\kappa_1 x} & & \psi_N(x) = A_N e^{i\kappa_N x} + B_N e^{-i\kappa_N x} \\ \phi_1 = -A_1 \begin{pmatrix} 1 \\ -1 \end{pmatrix} & & \phi_N = -A_N \begin{pmatrix} 1 \\ -e^{2i\kappa_N} \end{pmatrix} \end{array} \tag{10}$$

Here the idea is to find the eigen-energies with a root-finding algorithm. So we need a function $f(E)$ that is null when we have an eigen-function.

BJD notes suggest the relation between ϕ_N and $\tilde{\phi}_N$

$$\tilde{\psi}_N(x=1) \sim \tilde{\psi}_N(x=1) \implies \frac{\tilde{A}_N}{\tilde{B}_N} - \frac{1}{-e^{2i\kappa_N}} = 0 = f(E) \tag{11}$$

However, as we approach an eigen-energy, $f(E)$ varies its order of magnitude wildly, leading to asymptotes and fake roots.

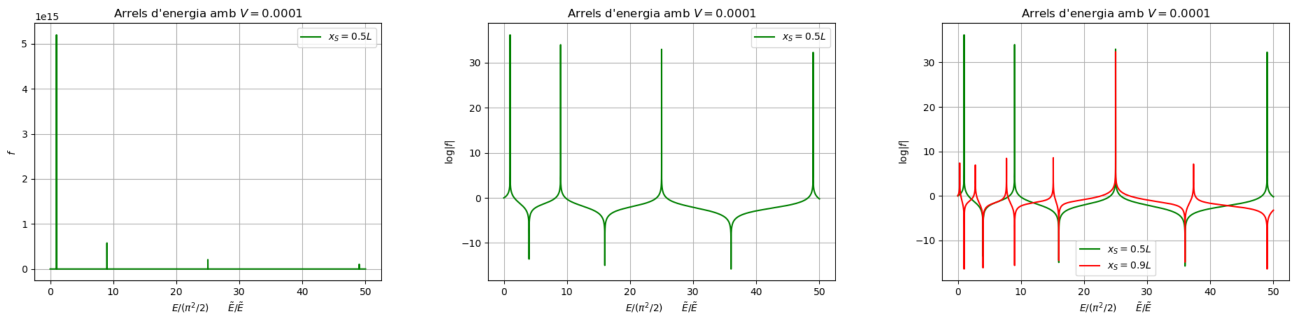

FIG. 1: Compute of (11) for a squared infinite potential, $N = 2$ $V_1 = 0$ $V_2 = 0$ and $x_1 = 0.5$. We expect to cut the horizontal axis on $1, 4, 9, 25, ...$. On the first one, the magnitude varies too much. We apply the logarithm on the second. But on the second one, there are asymtotes instead of roots. We change x_1 to 0.9 to see if they are really roots on the third. But on the third one there are fake roots.

An alternative function $f(E)$ that is null when we have an eigen-function can be the wave-function value at the right wall

$$\tilde{\psi}_N(x=1) = 0 = \tilde{A}_N e^{i\kappa_N} + \tilde{B}_N e^{-i\kappa_N} = f(E) \tag{12}$$

If V_N is smaller/bigger than E, $\tilde{\psi}_N$ will be real/imaginary. For increasing E, $\tilde{\psi}_N$ makes a transition from 'pure' real to 'pure' imaginary values. The " are because the other part is never really 0, it remain floating between $\pm 10^{-16}$, constantly crossing the axis.

This $f(E)$ is $\mathbb{R}\tilde{\psi}_N - \mathbb{I}\tilde{\psi}_N = 0$ in order to only cross the axis when one of the arts does it. $\mathbb{R} + \mathbb{I}$ is not used because at $E \sim V_N$ real and imaginary parts have different signs, and if added, at $E = V_N$ you can get an extra root.

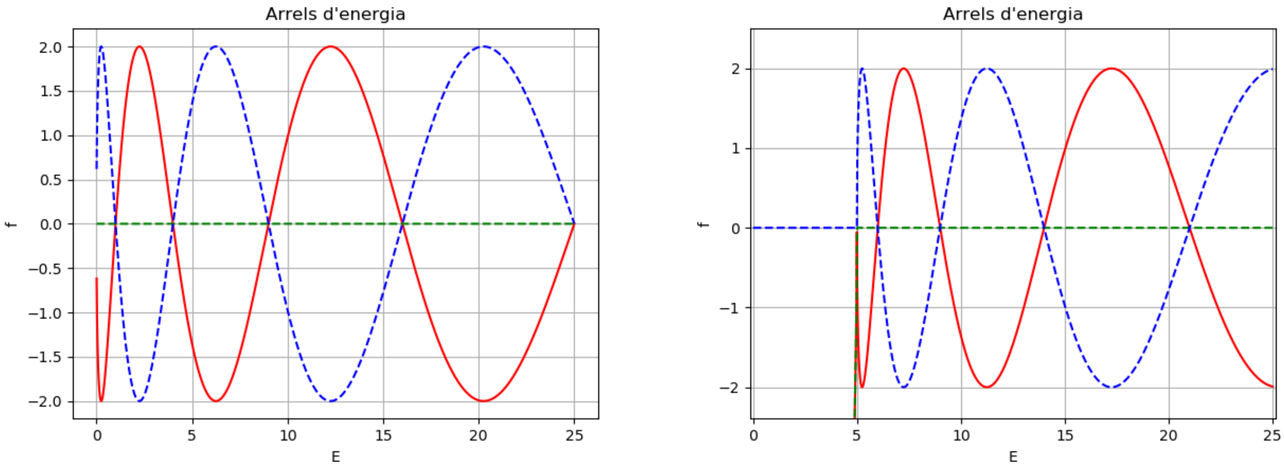

FIG. 2: Compute of (12). On the left, for a squared infinite potential $V_k = 0$ for $\forall k$. It cuts the horizontal axis on $1, 4, 9, 25, \ldots$. On the right, $V_k = 5$ for $\forall k$. It cuts the horizontal axis on $1+5, 2+5, 4+5, 16+5, \ldots$.