TRAINEESHIP REPORT 2018/19

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A. [Oct 23] Analytical solution of the Stepped Infinite Square Well

We consider the time independent 1D Schrödinger equation

$$-\frac{2m}{\hbar^2}(E-V)\Psi = \Psi''. \tag{1}$$

Given an infinite square potential of size L, with a discontinuity on $x_S teep$ dividing it into two regions

$$\begin{cases} V(x) = 0 & 0 < x < x_S \\ V(x) = V & x_S < x < L \\ V(x) = \infty & x = 0, L \end{cases} \tag{2}$$

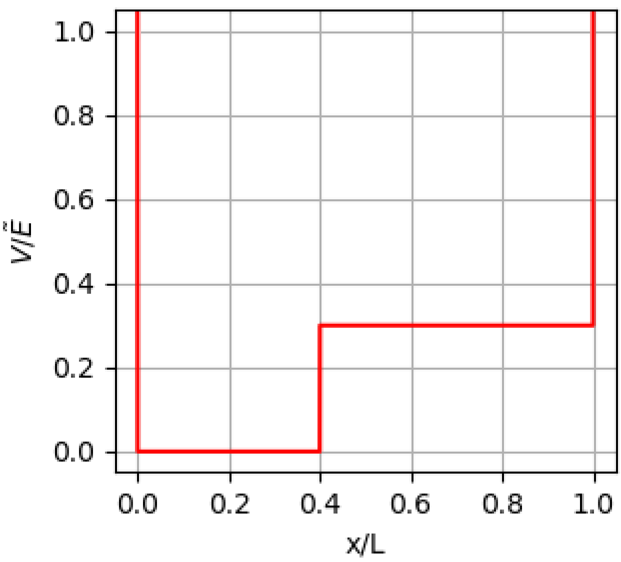


FIG. 1: Example of a well with a step of size $V = 0.3\tilde{E}$ and position $x_S = 0.4L$. Where L is the width of the well, and $\tilde{E}$ is an adequate energy unit defined at (11).

We will have a wave-function (wf) for each region

$$\begin{cases} \Psi_L(x) = A\exp(i\alpha x) + B\exp(-i\alpha x) & 0 < x \le x_S \\ \Psi_R(x) = C\exp(i\beta x) + D\exp(-i\beta x) & x_S < x < L \end{cases} \tag{3}$$

where,

$$\alpha = \sqrt{\frac{2m}{\hbar^2}E} \qquad\qquad \beta = \sqrt{\frac{2m}{\hbar^2}(E-V)} \tag{4}$$

The 4 parameters (A, B, C and D) of our wf are defined with 4 boundary conditions.

$$\begin{cases} \Psi_L(0) = \Psi_R(L) = 0 & \Rightarrow \begin{cases} A + B = 0 \\ C\exp(i\beta L) + D\exp(-i\beta L) = 0 \end{cases} \\ \Psi_L(x_S) = \Psi_R(x_S) = 0 \\ \Psi'_L(x_S) = \Psi'_R(x_S) = 0 \end{cases} \tag{5}$$

The two first equations describe the wf behavior at infinite walls. They leave each wf with only one constant.

$$\begin{aligned} \Psi_L(x) &= A(e^{i\alpha x} - e^{-i\alpha x}) \\ \Psi_R(x) &= Ce^{i\beta L}(e^{i\beta(x-L)} - e^{-i\beta(x-L)}) \end{aligned} \tag{6}$$

The other two equations demand continuity of both the wf and its derivative.

$$\begin{cases} A(e^{i\alpha x_S} - e^{-i\alpha x_S}) = Ce^{i\beta L}(e^{i\beta(x_S-L)} - e^{-i\beta(x_S-L)}) \\ i\alpha A(e^{i\alpha x_S} + e^{-i\alpha x_S}) = i\beta Ce^{i\beta L}(e^{i\beta(x_S-L)} + e^{-i\beta(x_S-L)}) \end{cases} \tag{7}$$

By multiplying and dividing we have two relations:

$$\begin{aligned} \frac{(e^{i\alpha x_S} - e^{-i\alpha x_S})}{i\alpha(e^{i\alpha x_S} + e^{-i\alpha x_S})} &= \frac{(e^{i\beta(x_S-L)} - e^{-i\beta(x_S-L)})}{i\beta(e^{i\beta(x_S-L)} + e^{-i\beta(x_S-L)})} \\ \alpha A^2(e^{2i\alpha x_S} - e^{-2i\alpha x_S}) &= \beta C^2 e^{2i\beta L}(e^{2i\beta(x_S-L)} - e^{-2i\beta(x_S-L)}) \end{aligned} \tag{8}$$

The first relation is between α and β. Given x_S and V, the eigenenergies of our system are the ones which satisfy this relation. And we can find them looking for roots on the function

$$f(\alpha,\beta,x_S) = f(E,V,x_S) = \frac{(e^{i\alpha x_S} - e^{-i\alpha x_S})}{i\alpha(e^{i\alpha x_S} + e^{-i\alpha x_S})} - \frac{(e^{i\beta(x_S-L)} - e^{-i\beta(x_S-L)})}{i\beta(e^{i\beta(x_S-L)} + e^{-i\beta(x_S-L)})} \tag{9}$$

We are calling this function the energy levels finder (elf).

The second relation is between the remaining parameters, A and C:

$$C^2 = \frac{\alpha(e^{2i\alpha x_S} - e^{-2i\alpha x_S}}{\beta e^{2i\beta L}(e^{2i\beta(x_S-L)} - e^{-2i\beta(x_S-L)})} A^2 \tag{10}$$

We can write C as a function of A, and then find A imposing normalization:

$$\begin{aligned} 1 &= \int_0^1 \Psi^*(x)\Psi(x)\,dx = \int_0^{x_S} \Psi_L^*(x)\Psi_L(x)\,dx + \int_{x_S}^1 \Psi_R^*(x)\Psi_R(x)\,dx \\ 1 &= A^2 \int_0^{x_S} \tilde{\Psi}_L^*(x)\tilde{\Psi}_L(x)\,dx + C^2 \int_{x_S}^1 \tilde{\Psi}_R^*(x)\tilde{\Psi}_R(x)\,dx \\ 1 &= A^2 \left[\int_0^{x_S} \tilde{\Psi}_L^*(x)\tilde{\Psi}_L(x)\,dx + \frac{\alpha(e^{2i\alpha x_S} - e^{-2i\alpha x_S}}{\beta e^{2i\beta L}(e^{2i\beta(x_S-L)} - e^{-2i\beta(x_S-L)})} \int_{x_S}^1 \tilde{\Psi}_R^*(x)\tilde{\Psi}_R(x)\,dx \right] \\ A &= \frac{1}{\sqrt{[...]}} \end{aligned} \tag{11}$$

B. [Oct 24] Testing the eigenenergies found

For V = 0 we have only one wf:

$$\Psi(x) = A\exp(ikx) + B\exp(-ikx) \tag{12}$$

$$\text{at: } 0 < x < L \qquad \text{with: } k = \sqrt{\frac{2m}{\hbar^2}E}$$

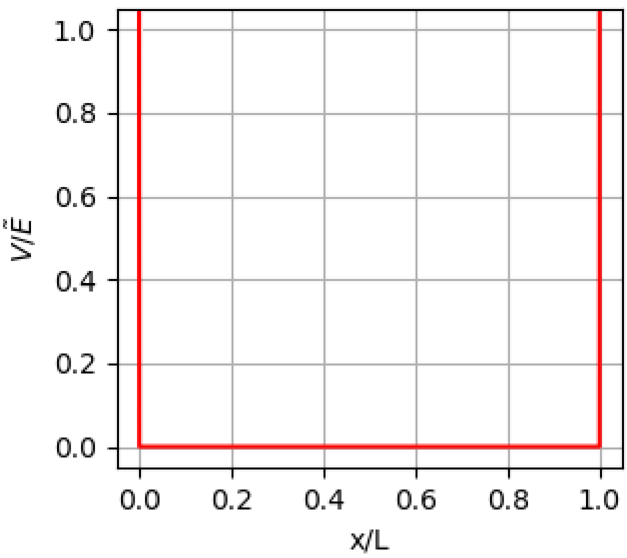


FIG. 2: Example of a squared infinite well. Where L is the length of the well, and $\tilde{E}$ is an adequate energy unit defined on the next section.

Now the only boundary conditions are at the walls:

$$\Psi(0) = \Psi(L) = 0 \quad \Rightarrow \quad \begin{cases} A + B = 0 \\ A\exp(ikL) + B\exp(-ikL) = 0 \end{cases} \tag{13}$$

We find the wave number

$$Ae^{ikL} - Ae^{-ikL} = 0 \quad \Rightarrow \quad e^{2ikL} = 1 = e^{2i\pi n} \quad \Rightarrow \quad \boxed{k = \frac{\pi n}{L} \quad \text{amb: } n \in \mathbb{N}} \tag{14}$$

And then we find both the eigenenergies and the adequate energy unit of the infinite squared well

$$k = \sqrt{\frac{2m}{\hbar^2}E} = \frac{\pi n}{L} \quad \Rightarrow \quad E = \frac{\hbar^2\pi^2 n^2}{2mL^2} = \frac{\pi^2 n^2}{2}\tilde{E} \tag{15}$$

Note that for $V = 0$ the energy of the well is proportional to its width:

$$E_{n=1}(V = 0) \propto \frac{1}{L^2} \tag{16}$$

For a well measuring half the width $L' = L/2$ we would have four times the energy $E' = 4E$.

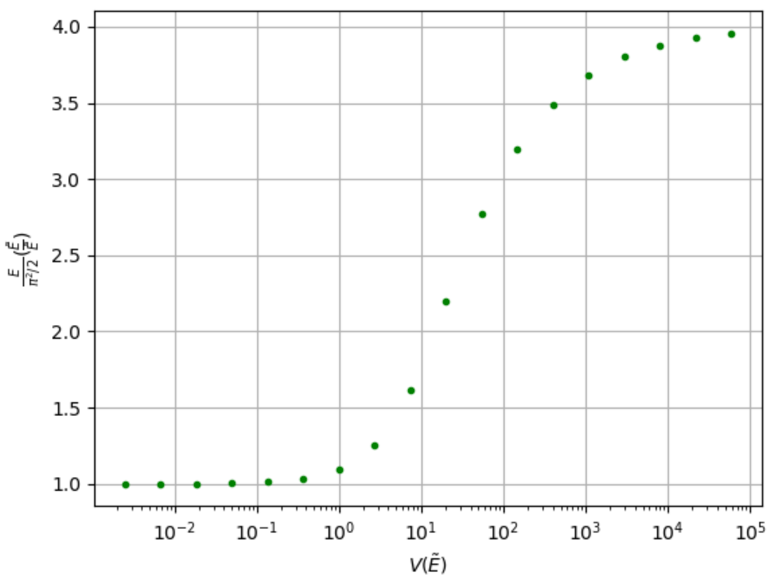


FIG. 3: Representations of the first energy level for different values of V. Here we double test the elf. For $V = 0$ we find the energy $E_{n=1} = (\pi^2/2)\tilde{E}$. And for $V \to \infty$ (which corresponds to the same squared infinite well with $V = 0$ but measuring half the width) we find 4 times the initial energy.

C. [Oct 29] Problems with the energy levels finder

From the previous figure, I figured out my elf was correct. So I carried on with the game, drawing the wf and the probability for $V \sim 0$.

The wf only depends on E, V and x_S, and it must satisfy the boundary conditions, as stated in the first section. For $V \sim 0$ and $x_S = 0.5L$ we find the first energy $E_{n=1}$, which corresponds to a 0-nodes sinus wave function. But if I move the step to $x_S = 0.9L$, the wf changes.

And it shouldn't change that much, since I'm moving a very thin step. Note that everything gets wider, almost as if we had a new $L' = 2L$. It's the opposite situation of the previous section, and we know it means there's a new energy level $E' = E/4$. A wrong one. So I got back to the elf.

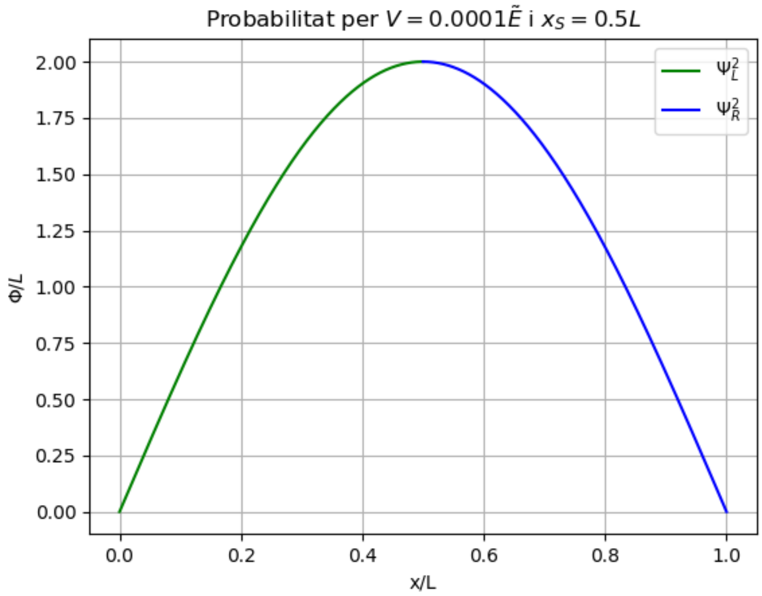


FIG. 4: Probability of a particle's position for $V \sim 0$ and $x_S = 0.5L$. Right and Left wf are continuous. It resembles the function it should be, a squared sinus. It means the energy found is right.

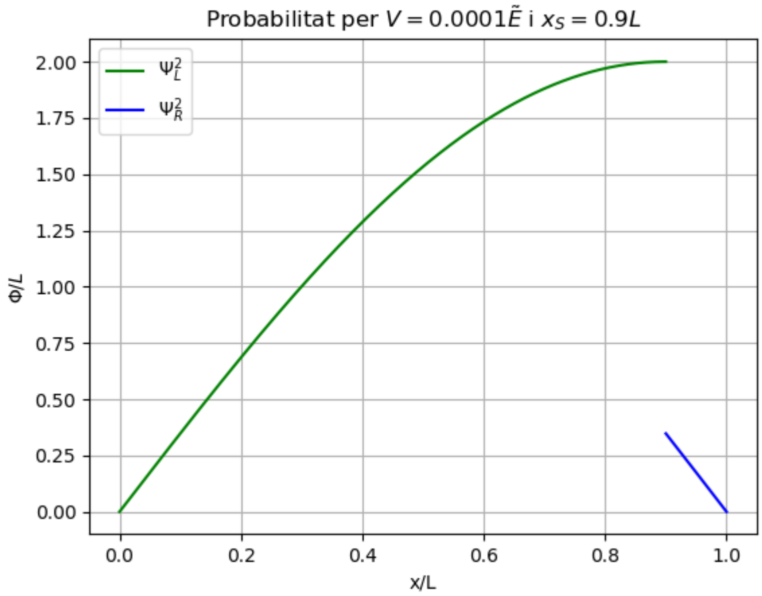


FIG. 5: Probability of a particle's position for $V \sim 0$ and $x_S = 0.9L$. There's a discontinuity, and both wf seem to be part of a much wider squared sinus. It means the energy is wrong.

D. [Nov 7] Refining the energy levels finder

The elf function (9) is a difference between two trigonometric functions:

$$f(\alpha, \beta, x_S) = f(E, V, x_S) = \frac{(e^{i\alpha x_S} - e^{-i\alpha x_S})}{i\alpha(e^{i\alpha x_S} + e^{-i\alpha x_S})} - \frac{(e^{i\beta(x_S - L)} - e^{-i\beta(x_S - L)})}{i\beta(e^{i\beta(x_S - L)} + e^{-i\beta(x_S - L)})}$$

When computing the elf function, values near the roots may diverge and even be complex due to overflow. The elf function is a real function. It is actually a difference between tangents.

$$f(E > V, x_S) = \frac{\tan(\alpha x_S)}{\alpha} - \frac{\tan(\beta(x_S - L))}{\beta}$$
$$f(E < V, x_S) = \frac{\tan(\alpha x_S)}{\alpha} - \frac{\tanh(\beta(x_S - L))}{\beta} \tag{17}$$

To avoid this, we can reformulate the function it as a fraction between the two elements

$$f'(E > V, x_S) = \frac{\beta \tan(\alpha x_S)}{\alpha \tan(\beta(x_S - L))} - 1 = 0 \tag{18}$$

E. [Nov 19] Finishing the simple potential

We can se that the program computes the ground state of a given potential.

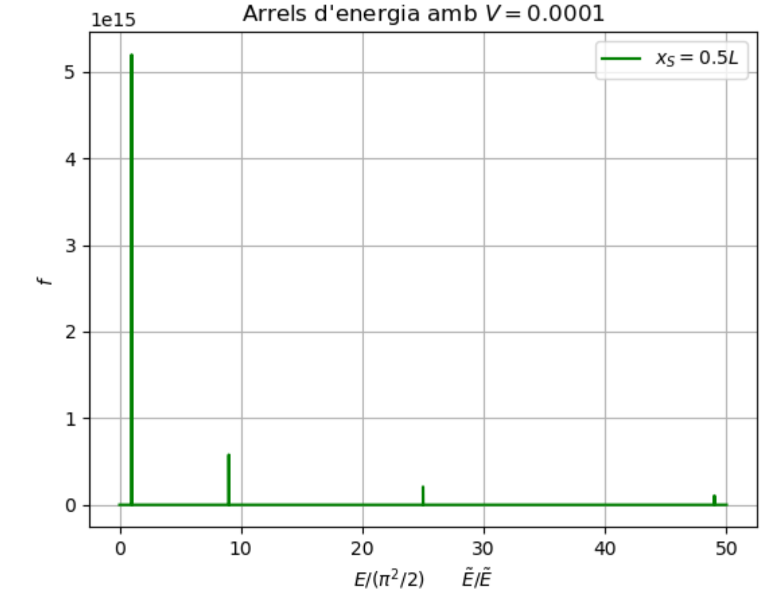


FIG. 6: The elf as a function of E, for $V \sim 0$ and $x_S = 0.5L$ (the step that works). The energy levels finder is a function that has its roots on the eigenenergies. Representing the raw function only illustrates there are huge overflows near the roots. We cannot actually see were the function crosses the abscissa.

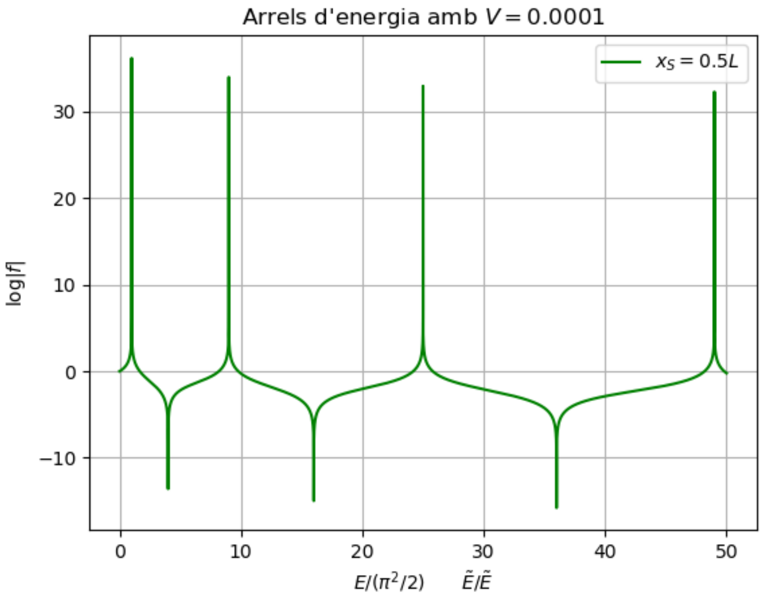
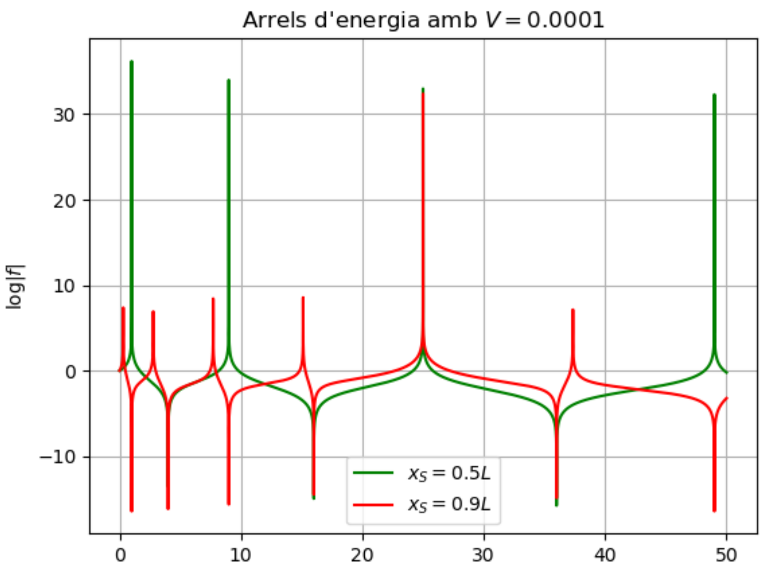
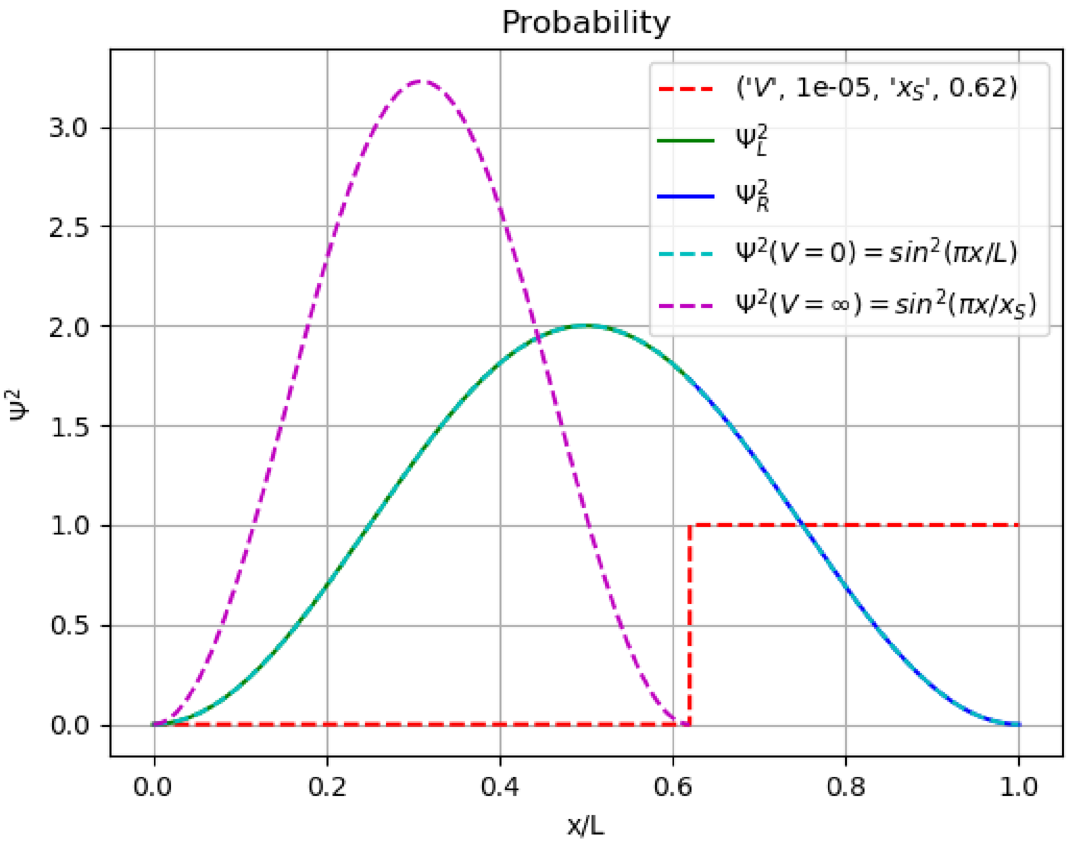


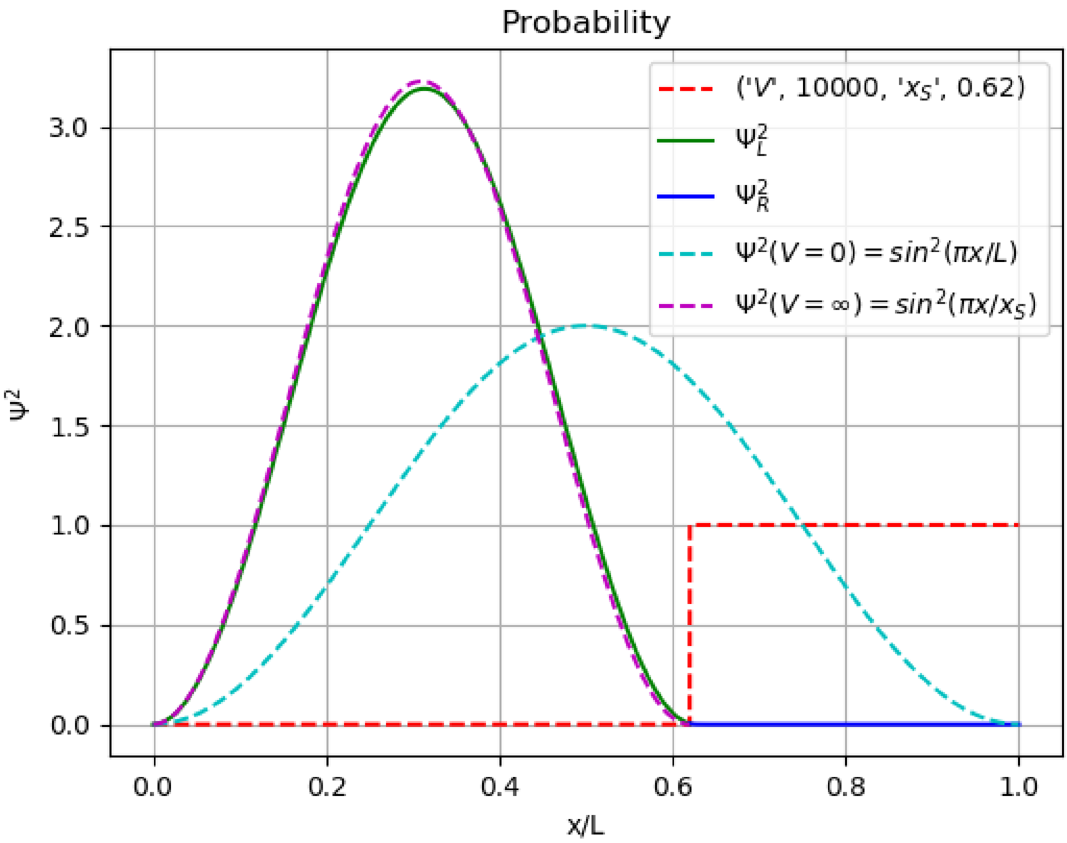
FIG. 7: The logarithm of the elf as a function of E, for $V \sim 0$ and $x_S = 0.5L$ (the step that works). It has the eigenenergies on its peaks. We identify $[E_{n=2}, E_{n=3}, E_{n=4}, ...] = [4, 9, 16...]E_{n=1}$ there.





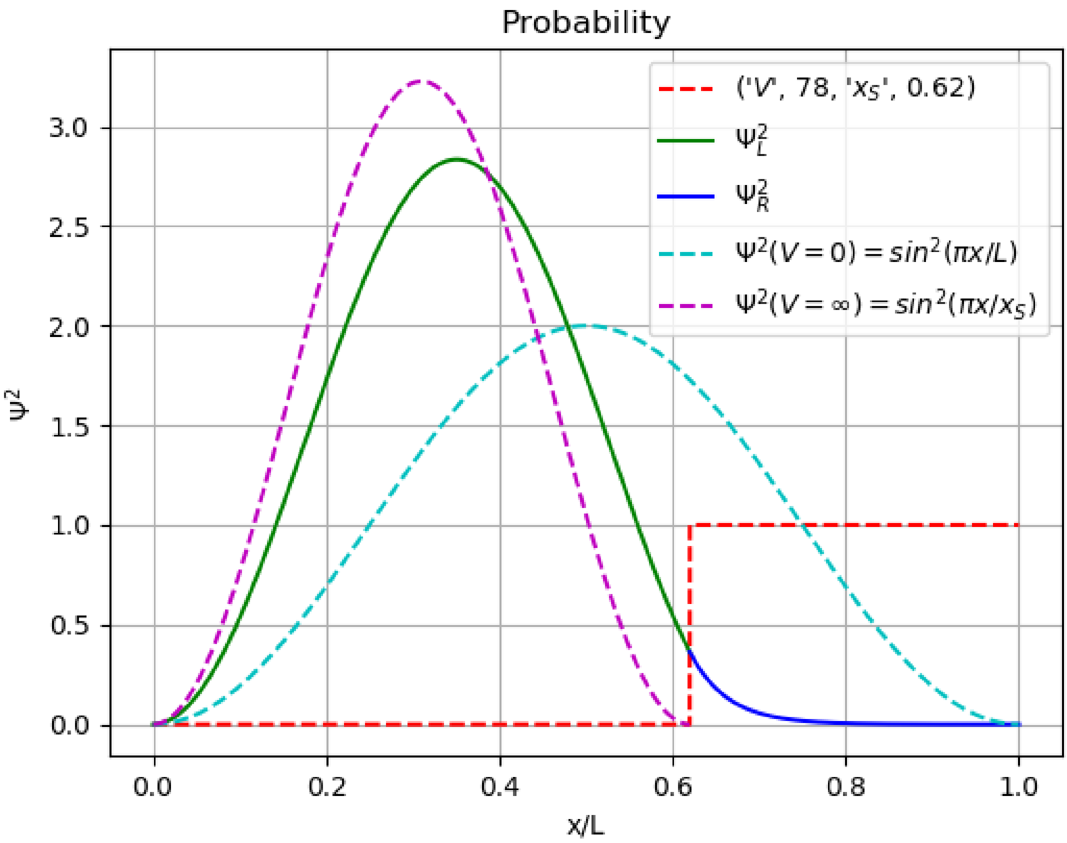
V.png

FIG. 9: The ground state of our a small stepped potential. This is an example of how a small potential, in this case $V = 10^-5$, is like no step at all (the wider sinusoidal solution represented in discontinued lines).



V.png

FIG. 10: The ground state of our a potential with a big step. Note how a big potential, in this case $V = 10^4$, is like a wall on x_S (the narrower sinusoidal solution represented in discontinued lines).



V.png

FIG. 11: The ground state of an intermediate potential. The solution is "in between" the two extremal solutions.