ETH
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# Computational Quantum Physics
# Exercise 1

FS 16
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**Problem 1.1 1D quantum scattering problem**

We consider a particle in one dimension, which is scattered at a potential barrier. This problem can be numerically solved using the Numerov algorithm.
Proceed as described in the lecture notes in section 3.1.2.

1. Debug your code by using a rectangular potential

$$V(x) = \begin{cases} 1, & 0 < x \leq a \\ 0, & \text{else} \end{cases} . \tag{1}$$

   (a) Fix a value of the energy $E \in [0, V]$ and compute the transmission probability $T = 1/|A|^2$.

   (b) For this potential an exact solution is known:

$$T = \frac{1}{1 + \frac{V^2 \sinh^2(\kappa a)}{4E(V-E)}}, \tag{2}$$

   with $\kappa = \sqrt{2m(V-E)}/\hbar$. Check how well you can reproduce $T(a)$ by varying the discretization used for Numerov.

2. Now use your code to simulate a parabolic potential barrier that is not analytically solvable

$$V(x) = \begin{cases} 4\left(\frac{x}{a} - \frac{x^2}{a^2}\right), & 0 < x \leq a \\ 0, & \text{else} \end{cases} . \tag{3}$$

   (a) Check that the results is converged by running a few values of the discretization.

   (b) Compare the result obtained for the parabolic potential with the rectangular potential. Does it match your expectations?

3. Next we want to look at the fourth order potential

$$V(x) = \begin{cases} 4\left((\frac{x-a/2}{a/2})^2 - (\frac{x-a/2}{a/2})^4\right), & 0 < x \leq a \\ 0, & \text{else} \end{cases} . \tag{4}$$

   (a) Investigate the dependence of $T(a)$ on the energy for different $a \in (0, 4]$.

   (b) Explain the physical reasons for this behaviour of the transmission coefficient.

This dependency $T(a)$ plays a crucial role for the realization of the scanning tunneling microscope (STM). [Review of Modern Physics **59**, 615 (1987). Nobel prize 1986.]