Dynamics of a particle in various 1D potentials

In this assignment you will discretize both space and time in order to compute the dynamics of a quantum wavepacket in the presence of a variety of one-dimensional environments, each represented as a different potential energy as a function of position, $V(x)$.

Throughout this assignment, you are encouraged to vary the parameters of the simulation in order to more easily "see what is going on" for each scenario!

Part 1: FFT

You have been provided a Jupyter notebook to use as a template. Near the bottom of this notebook, a function is defined for you named "transform" that computes $\Psi(k,t)$. Add detailed comments throughout this function to describe how $\Psi(k,t)$ is being computed.

Part 2: Empty Box

Make sure that you are able to execute all of the code in this notebook. Explore what happens for different values of the parameters using a "particle in a box" with $V(x) = 0$ for all $0 < x < L$. (You are already given the code for this in the notebook.)

Generate some results, and discuss your results. What happens? Why does it make sense?

Part 3: Uniform Field

Turn on a uniform electric field, $\epsilon = +10$ Volts/nanometer, and simulate the dynamics of an electron that is subjected to this field. (You may call the functions that have been given to you as they are written. Adding the electric field doesn't take much code!) Again, play with the parameters in order to more easily see what is going on. Discuss your results.

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Part 4: Finite Barrier

Consider an electron that is inside of a well with a narrow *repulsive* region of width w in the middle of a box of width L. The potential energy would be described by

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < \frac{L}{2} - \frac{w}{2} \\ +V_0 & \text{for } \frac{L}{2} - \frac{w}{2} \le x \le \frac{L}{2} + \frac{w}{2} \\ 0 & \text{for } \frac{L}{2} + \frac{w}{2} < x < L. \end{cases}$$

Simulate an electron traveling toward, and interacting with, this repulsive region. Explore what happens as you vary the strength of the repulsion and the width of the repulsive region. Discuss your results. What is the physical significance of your results?

Part 5: Finite Well

Repeat Part 4, but this time using an attractive region in the middle of the well:

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < \frac{L}{2} - \frac{w}{2} \\ -V_0 & \text{for } \frac{L}{2} - \frac{w}{2} \le x \le \frac{L}{2} + \frac{w}{2} \\ 0 & \text{for } \frac{L}{2} + \frac{w}{2} < x < L. \end{cases}$$

Again, discuss your results!