

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

5.73 Quantum Mechanics I Fall, 2018

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Problem Set #1

Reading: C-TDL, pages 9-39, 50-56, 60-85

Problems:

1. This question is based on Figure 1 of Complement J_I CTDL p84. This is a problem that involves many repeated calculations; thus it is best done using a computer. Since computers like pure numbers, it is convenient to express the problem in dimensionless quantities and then, if necessary, express the final result in the appropriate units. One very effective and widely used way to do this is to use “atomic units”:

mass = m_e	mass of electron
charge = e	charge of electron
length = $1a_0$	(Bohr radius)
action = $h / 2\pi = \hbar$	(energy times time or length times momentum)
energy = E_h	(1 Hartree)

Every dimensioned quantity, Q , in an equation is converted to a pure number by dividing it by the appropriate atomic unit quantity (expressed in the same units as the quantity of interest), denoted by:

$$\hat{Q} = Q / Q \text{ (atomic unit)}$$

$$\hat{m} = m / m_e$$

$$\hat{q} = q / e$$

$$\hat{x} = x / a_0$$

$$\hat{\hbar} = \hbar / \hbar = 1$$

$$\hat{E} = E / E_h.$$

The 1-dimensional Schrödinger equation becomes

$$\left[-\frac{1}{2\hat{m}} \frac{d^2}{d\hat{x}^2} + \frac{1}{E_h} V(\hat{x}) - \hat{E} \right] \psi(\hat{x}) = 0$$

Let $\hat{m} = 1$ (i.e., an electron)

$$\hat{V} = 1.0 \times 10^{-3} \text{ (about kT at 300K).}$$

- A. Solve the problem for a Gaussian wavepacket of the generic form

$$G(x; x_0, \Delta x) = (2\pi)^{-1/2} \frac{1}{\Delta x} e^{-(x-x_0)^2/[2(\Delta x)^2]}$$

incident from the left on a step potential of step-height \hat{V}_0 . Choose the average energy of the wavepacket to be $\hat{E} = 1.05\hat{V}_0$ and the variance of the Gaussian wavepacket to be

$$(\Delta\hat{x})^2 = \frac{1}{4(\Delta\hat{k})^2}$$

where

$$\Delta\hat{k} = [0.1\hat{V}_0]^{1/2}.$$

Convert this simple Gaussian in \hat{x} to a Gaussian wavepacket in \hat{k} which is localized at $\hat{x}_0 = 10\Delta\hat{x}_0$ to the left of the barrier. To get a sense of how this Gaussian wavepacket scatters off of the potential step you would ideally make a movie of $|\Psi(\hat{x}, \hat{t})|^2$ vs. \hat{x} sampled at a series of values of \hat{t} .

$$\Psi(\hat{x}, \hat{t}) = \int d\hat{k} g(\hat{k}) e^{i\alpha(\hat{k})} e^{i\hat{k}\hat{x}} e^{-i\hat{E}(\hat{k})\hat{t}}$$

where $g(\hat{k})e^{i\alpha(\hat{k})}$ is the \hat{k} -dependent complex amplitude of your Gaussian wavepacket localized at $\hat{x}_0 = \hat{x}(\hat{t} = 0)$. To make your task easier, sample this complex amplitude at the 5 values of \hat{k} : \hat{k}_0 , $\hat{k}_0 \pm \Delta\hat{k}$, and $\hat{k}_0 \pm 2\Delta\hat{k}$ and approximate $\Psi(\hat{x}, \hat{t})$ by a sum over the five wavefunctions, $\Psi_{\hat{k}}(\hat{x}, \hat{t})$, rather than the integral. To make it even easier, sample at 5 values of \hat{t} . These 5 values of \hat{t} should be $\hat{t} = 0$, the time when the center of the wavepacket is at the barrier \hat{t}_{barrier} , $0.9\hat{t}_{\text{barrier}}$, $1.1\hat{t}_{\text{barrier}}$, and $2\hat{t}_{\text{barrier}}$.

Now use your “movie” results to answer the following questions about the wavepacket incident on a step.

- B. What is happening in part C of Figure 1? What are the fringes at $x < 0$? Why are there no fringes at $x > 0$? What change in E and/or m would cause the fringe spacing to double? What controls the modulation depth (define this any way you think reasonable) of the fringes?
- C. What is happening in part D of the figure? What controls the relative areas of the two peaks? Are there any resonances in the ratio of the areas of the transmitted and reflected peaks? If there are no resonances, why not? If there is a resonance, what feature of the potential is responsible for it?
- D. The left and right peaks in part D have different widths and are centered at different distances from $x = 0$. Why?

- E. Suppose you know that there is a step barrier but not where it is or how high it is. Describe the experiments you would do to determine the distance from x_0 to the barrier and the actual value of V_0 .
- F. How would you expect scattering from an infinite length step:

$$\begin{aligned} V(x) &= 0 & x < 0 \\ V(x) &= V_0 & x \geq 0 \end{aligned}$$

and a finite length symmetric step:

$$\begin{aligned} V(x) &= 0 & x < 0, x > x_0 \\ V(x) &= V_0 & 0 \leq x \leq x_0 \end{aligned}$$

to differ? What is the most salient distinguishing feature of the scattering? How would you determine the height and length of the finite step in the minimum number of observations? If the step is not symmetric

$$\begin{aligned} V(x) &= 0 & x < 0 \\ V(x) &= V_0 & 0 \leq x \leq x_0 \\ V(x) &= V_0/2 & x > x_0, \end{aligned}$$

how would you experimentally distinguish the non-symmetric step from the symmetric step?

2. C-TDL, page 86, #2.
3. C-TDL, page 89, #7.

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