# Quantum Physics 1 - Homework 4

Due on Monday Oct 3, 12AM

**1. Wavepacket Scattering and the Plane-Wave Approximation** [9pt.]

In class, reflection and transmission coefficients ($R$ and $T$) are derived using plane waves. Using plane waves as wavefunctions is convenient from a mathematical viewpoint, but very awkward at the same time, since they are not normalizable. More realistic is to consider a Gaussian wavepacket scattering off a potential. Such a wavepacket is normalizable, but its evolution cannot be solved for analytically. Computer simulations of wavepackets scattering on a potential barrier are shown in class (see also `GWP-scattering-k271.mp4` attached).

In the exercise, you will investigate how well the plane-wave approximations for $R$ and $T$ compare to numerical simulations of Gaussian wavepackets scattering off a potential barrier. Throughout, set $\hbar \equiv 1$ (so momenta $k$ and wavenumbers become equivalent) and take the mass of the particle to be $m = 1/2$. The kinetic energy of the particle is then $E(k) = \hbar^2 k^2/2m = k^2$. These units are used in the simulation as well.

### Gaussian wavepackets

In the simulation, the initial wavefunction has the form:

$$\psi(x, t = 0) = (\pi\sigma_0^2)^{-1/4}\, e^{-(x-x_0)^2/2\sigma_0^2}\, e^{ik_0 x},$$

and is called a Gaussian wavepacket since the probability density $|\psi|^2$ is a Gaussian. Its standard deviation is $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sigma_0/\sqrt{2}$, which gives a measure of the 'spread' of the wavefunction. The initial momentum space wavefunction $\phi(k, t = 0)$ can be obtained by taking the Fourier transform[1] of $\psi(x, t = 0)$, the result is:

$$\phi(k, 0) = (\sigma_0^2/\pi)^{1/4}\, e^{-\sigma_0^2(k-k_0)^2/2}\, e^{-i(k-k_0)x_0},$$

which again corresponds to the distribution $|\phi|^2$ being a Gaussian. Here $k_0$ is the average momentum or expectation value of the distribution.

a) (1.5pt) Compute the spread in momentum $\Delta k = \sqrt{\langle k^2\rangle - \langle k\rangle^2}$. Comment on the resulting product $\Delta x\, \Delta k$.

   *Hint:* To compute the integrals, you can set $k_0 \equiv 0$ without loss of generality. The following integral is useful:

$$\int_{-\infty}^{+\infty} dx\, x^2\, e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}\,\frac{1}{2\alpha}.$$

[1] The Fourier transform is defined as:

$$\phi(k, t = 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x)\, e^{-ikx}\, dx.$$

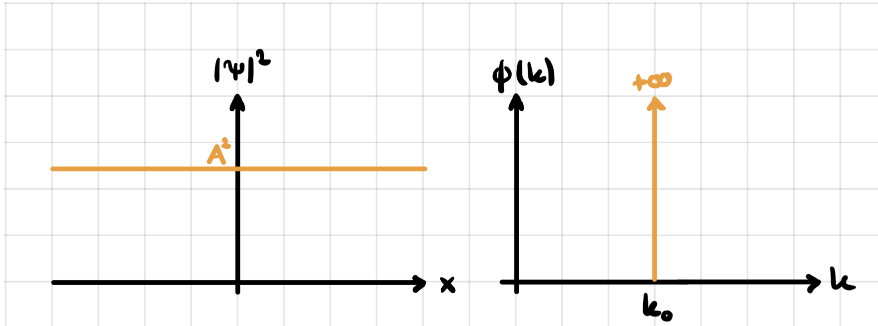


Figure 1: Left: $|\psi|^2(x)$. Right: $\phi(k)$.

First we compute $\langle k \rangle$ (with $k_0 = 0$):

$$\langle k \rangle = \int_{-\infty}^{\infty} dk\ k|\phi|^2 = 0,$$

since $k$ is an odd function and $|\phi|^2 \propto e^{-\sigma_0^2 k^2/2}$ is even and the product is odd, yielding zero. Now consider $\langle k^2 \rangle$, which gives:

$$\langle k^2 \rangle = \int_{-\infty}^{\infty} dk\ k^2|\phi|^2 = \sqrt{\frac{\sigma_0^2}{\pi}} \int_{-\infty}^{+\infty} dk\ k^2\ e^{-\sigma_0^2 k^2} = \sqrt{\frac{\sigma_0^2}{\pi}} \sqrt{\frac{\pi}{\sigma_0^2}} \frac{1}{2\sigma_0^2} = \frac{1}{2\sigma_0^2}.$$

Then $\Delta k = 1/\sqrt{2}\sigma_0$. The product $\Delta x\ \Delta k = 1/2$, which means that the wavepacket *hits* (saturates) the Heisenberg uncertainty principle (recall that $\hbar = 1$), this is a well-known property of Gaussian wavepackets.

## Plane Waves

For plane-waves, $\Delta x$ and $\Delta k$ become less well-defined, since they are not normalizable. However, to get a better feeling for the regime in which plane waves become reasonable *approximations* to well-defined wavepackets, you will take a stubborn attitude and give meaning to $\Delta x$ and $\Delta k$ anyway.

b) Consider a plane wave of the form $\psi(x) = A\ e^{ik_0 x}$.

   i) (0.5pt) Sketch the probability density $|\psi|^2$ as a function of $x$.
   The sketch should be a horizontal line at height $A^2$ above the $x$-axis, essentially spanning the entire axis (from $x = -\infty$ to $x = +\infty$). See Fig. 1 (left).

   ii) (0.5pt) Based on the sketch, what is the 'spread' $\Delta x$? No calculation required; a qualitative answer suffices.
   From the sketch, you see that $|\psi|^2$ spreads along the entire $x$-axis, so that $\Delta x$ is practically infinite for a plane wave: $\Delta x \to \infty$.

   iii) (0.5pt) How does this spread compare to the wavelength $\lambda_0 = 2\pi/k_0$ of the plane wave?
   The spread $\Delta x$ is much much larger than the wavelength $\lambda_0$, which we assume to be finite: $\Delta x \gg \lambda_0$.

c) The momentum space wavefunction $\phi(k)$ is related to $\psi(x)$ via the Fourier transform.

i) (0.5pt) Show that for the plane wave above, $\phi(k)$ is proportional to a Dirac delta function located at $k = k_0$.

The Dirac delta function $\delta(k)$ is given by:

$$\delta(k) = \int \frac{dx}{2\pi}\, e^{-ikx}.$$

Inserting $\psi(x) = A\, e^{ikx}$ into the Fourier transform, we find:

$$\phi(k) = A \int \frac{dx}{\sqrt{2\pi}}\, e^{-i(k-k_0)x} = A \times \sqrt{2\pi}\, \delta(k-k_0) \propto \delta(k-k_0).$$

ii) (0.5pt) Sketch $\phi(k)$ as a function of $k$.

Since the incident wave is travelling in the positive $x$ direction, we have $k_0 > 0$ and the sketch should be a spike, representing the Dirac delta function, at $k = k_0$. See Fig. 1 (right).

iii) (0.5pt) What is the 'spread' $\Delta k$? Again, a qualitative answer suffices.

The Dirac delta function is an infinitely thin spike with essential no spread, so $\Delta k \to 0$.

iv) (0.5pt) How does this spread compare to the momentum $k_0$?

Assuming $k_0$ is finite, we have $\Delta k \ll k_0$ or $\Delta k / k_0 \to 0$.

**Simulations**

In the simulations, like in video `GWP-scattering-k271.mp4`, Gaussian wavepackets with $\sigma_0 = 0.05$ and momenta $k_0$ in the range $150 - 750$ impinge a rectangular potential barrier of height $V_0 = 63170$ and width $w = 0.021$.

d) (2pt) Watch `GWP-scattering-k271.mp4` and estimate the approximate values of the transmission and reflection coefficients from the graphs (one digit accuracy suffices). After scattering on the potential well, the initial wavepacket (which is normalized to have unit area) splits into the transmitted and reflected wavepackets. Integrating over the area of these wavepackets gives us the transmission and reflection coefficients. These automatically satisfy $R + T = 1$ since the initial wavepacket is normalized and probability is conserved. From a first glance, these are roughly $R = 2/3$ and $T = 1/3$.

The dataset `kRdata.csv` contains reflection coefficients (second column) numerically determined in the simulation for a large number of momenta $k_0$ equally spaced in the range $150 - 750$ (first column). Import the dataset into a python notebook and visualize it in a *scatter* plot, the result should look something like Fig. 2 below.

e) (2pt) Look up the reflection coefficient $R$ for scattering of plane waves off a potential barrier as a function of momentum $k_0$. Add it as a continuous curve to the plot. This question only requires the resulting plot; no code or formulae are needed. Please add your name(s) to the legend of the plot.

*Hint:* Be careful with the two different regimes $k_0^2 < V_0$ and $k_0^2 > V_0$! Recall that we use units where $\hbar = 1$ and $m = 1/2$.

For scattering states, with $E = k_0^2 > V_0$, we have:

$$R_{\text{scat}} = 1 - \frac{1}{1 + V_0^2 \sin^2(k_1 w)/[4E(E - V_0)]},$$

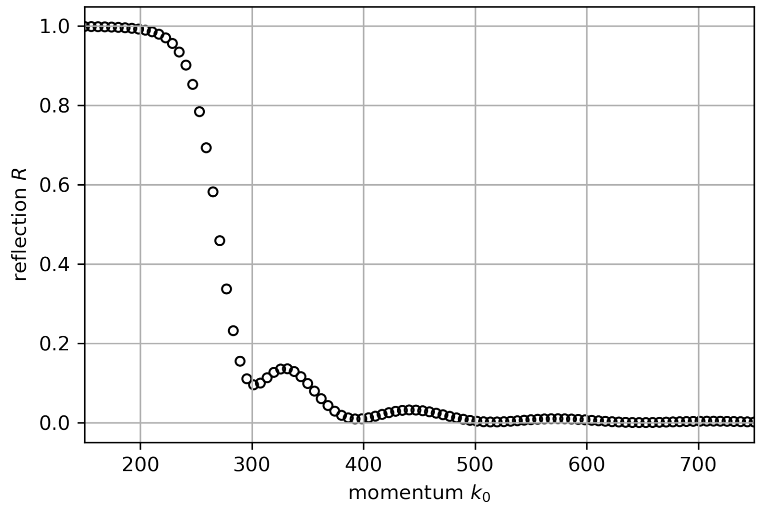


Figure 2:

where $k_1 = \sqrt{E - V_0}$. For bound states, with $k_0^2 < V_0$, we have:

$$R_{\text{bound}} = 1 - \frac{1}{1 + V_0^2 \sinh^2(k_1 w)/[4E(V_0 - E)]},$$

where $k_1 = \sqrt{V_0 - E}$. In the simulation, the turnover point between the two solutions occurs at $k_0 = \sqrt{V_0} \simeq 251$. See the curve in blue in the plot. To correctly plot this, one makes an array with $k_0$ values spanning from 150 to 251 and evaluates $R_{\text{bound}}$ on array values. For the range 251 to 750 one does the same, but now using $R_{\text{scat}}$.

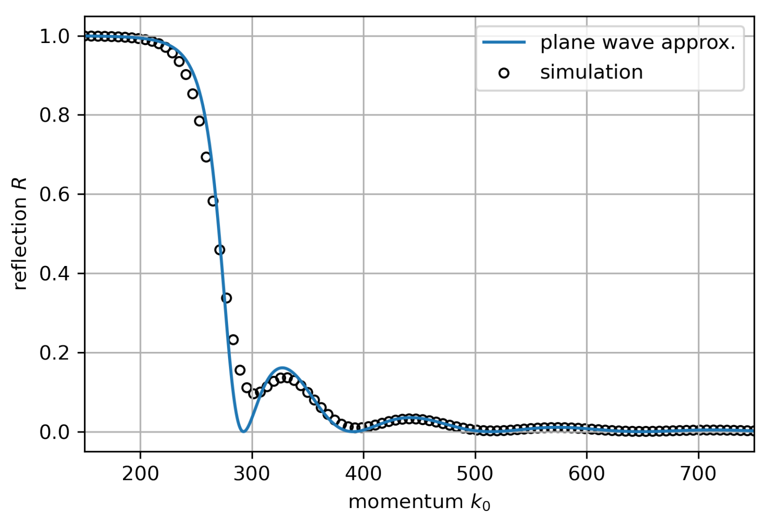


Figure 3:

You should find that the plane wave curve agrees well with the simulation data for $k_0 \gtrsim 400$ as well as for $k_0 \lesssim 200$.

f) (1pt) From your answers at b) and c), explain why the plane-wave curve and simulation data agree more and more as the momentum increases.

Given that $\sigma_0 = 0.05$, we have $\Delta k \simeq 14.14$ so that $\Delta k/k_0 = 14.14/k_0$. Therefore you see that as the momentum $k_0$ increases, the ratio $\Delta k/k_0$ becomes smaller and smaller, making the wavepackets better and better approximated by plane waves. In the plot produced in e), we indeed find that as $k_0$ increases beyond $k_0 \gtrsim 400$, the blue curve matches the simulation data very well since the plane wave-approximation becomes applicable there.