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:

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

Plane Waves

For plane-waves, Δx and Δk 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 Δx and Δk 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.

   ii) (0.5pt) Based on the sketch, what is the 'spread' Δx? No calculation required; a qualitative answer suffices.

   iii) (0.5pt) How does this spread compare to the wavelength $\lambda_0 = 2\pi/k_0$ of the plane wave?

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 $k = k_0$.

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

   iii) (0.5pt) What is the 'spread' Δk? Again, a qualitative answer suffices.

   iv) (0.5pt) How does this spread compare to the momentum k_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).

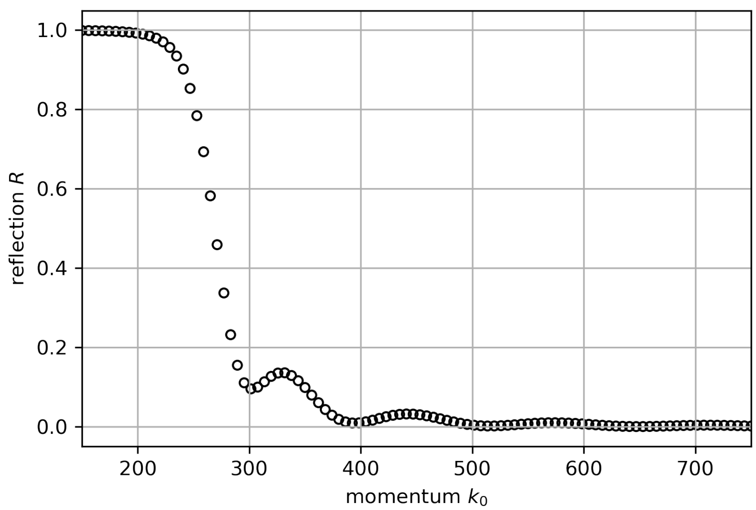
The dataset `kRdata.csv` contains reflection coefficients (second column) numerically determined in the simulation for a large number of momenta k_0 equally spaced in the range $150 - 750$ (first column). Import the dataset into a python notebook and visualize it in a *scatter* plot, the result should look something like Fig. 1 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 $m = 1/2$.

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.



1.0
0.8
0.6
0.4
0.2
0.0
reflection R
200
300
400
500
600
700
momentum k_0

Figure 1: