Problem 1: Wave-Packet in 1-D Box

We start by defining suitable dimensionless parameters. We choose \( a = 1, \hbar = 1, \tau = \frac{8\pi m a^2}{\hbar^2} = 1 \). This implies \( m = \frac{\pi^2}{8} \) and \( E_n = n^2 \).

i) With the above choice of parameters, the range of \( E \) is \( E = [2.5, 6.5] \) and \( \sigma \) is given to be 0.5. We evaluate the wavefunction as a function of \( x \) for different values of \( t \). For this purpose we use Mathematica to evaluate eqn.(3.113) of the lecture notes with \( \psi(x_0, t_0) \) given by eqn.(3.115) of the notes. The integrations are carried out numerically and 16 terms are retained in the sum.

ii) For this part \( k_0 = \pi \) with the present choice of units. \( \sigma \) is taken as 0.2.

Figure 1: (i)
Problem 2: Particle in 2-dimensional box

The stationary states wave function are determined by the time-independent Schrodinger equation.

\[- \frac{\hbar^2}{2m} (\partial_x^2 + \partial_y^2) \phi_E(x, y) = E \phi_E(x, y)\]

Since the Hamiltonian is a sum of operators each dependent only on a single variable (viz. x or y), one can express

\[\phi(x, y) = \phi_1(x)\phi_2(y)\]

where,

\[- \frac{\hbar^2}{2m} \partial_x^2 \phi_1(x) = E_1 \phi_1(x)\]
\[- \frac{\hbar^2}{2m} \partial_y^2 \phi_2(y) = E_2 \phi_2(y)\]

with \(\phi_1(\pm a) = 0 = \phi_2(\pm a)\) and \(E_1 + E_2 = E\)
We note that the box is symmetric with respect to the origin. Hence, the solutions obey this symmetry as well. Proceeding as in the one-dimensional case we define two types of solutions for $\phi^1(x), \phi^2(y)$:

- the even solution $\phi^{(e)}_E(x) = A_1 \cos k_1 x \phi^{(e)}_E(y) = A_2 \cos k_2 y$
- the odd solution $\phi^{(o)}_E(x) = A_1 \sin k_1 x \phi^{(o)}_E(y) = A_2 \sin k_2 y$

As derived in the lecture notes the boundary conditions imply that $k_1$ and $k_2$ can take only discrete set of values $k_n, n \in \mathbb{N}$.

$k_n = \frac{n\pi}{2a}, n = 1, 3, 5, \ldots$ for even solutions

and $k_n = \frac{n\pi}{2a}, n = 2, 4, 6, \ldots$ for odd solutions

The corresponding energy values are given by

$E_n = \frac{\hbar^2 \pi^2}{8ma^2} n^2, n = 1, 2, 3, \ldots$

With this $\phi^1(x), \phi^2(y)$ take the form

$$
\phi^{1(e)}_n(x) = A_1 n \cos \frac{n\pi x}{2a}
$$

$$
\phi^{2(e)}_n(y) = A_2 n \cos \frac{n\pi y}{2a}
$$

$$
\phi^{1(o)}_n(x) = A_1 n \sin \frac{n\pi x}{2a}
$$

$$
\phi^{2(o)}_n(y) = A_2 n \sin \frac{n\pi y}{2a}
$$

Normalisation of the wave functions implies $A_1 = A_2 = \sqrt{\frac{\pi}{a}}$. Thus the complete wave functions are give by

$$
\phi_{n_1, n_2}(x, y) = \frac{1}{a} \left\{ \begin{array}{ll}
\cos \frac{n_1 \pi x}{2a} \cos \frac{n_2 \pi y}{2a} & \text{for } n_1, n_2 = 1, 3, 5, \ldots \\
\sin \frac{n_1 \pi x}{2a} \sin \frac{n_2 \pi y}{2a} & \text{for } n_1, n_2 = 2, 4, 6, \ldots
\end{array} \right.
$$

with energy

$$
E_{n_1, n_2} = \frac{\hbar^2 \pi^2}{8ma^2} (n_1^2 + n_2^2), n_1, n_2 = 1, 2, 3, \ldots
$$

**Symmetries**

A 2-d box containing a particle has the following symmetries:

1. Rotation by $\pi$ about x and y axis. This has been exploited in deriving the stationary states.

2. Since the sides are equal a rotation by $\pi/2$ also leaves the system unaltered. This additional symmetry is reflected in the degeneracy of the energy levels.
\[
\begin{array}{|c|c|c|}
\hline
n_1, n_2 & \dfrac{E}{\hbar c^2 \pi^2 \mu a^2} & \text{degeneracy} \\
\hline
1,1 & 2 & \text{single} \\
1,2 & 5 & \text{two-fold} \\
2,2 & 8 & \text{single} \\
1,3 & 10 & \text{two-fold} \\
2,3 & 13 & \text{two-fold} \\
\hline
\end{array}
\]

**Problem 3: Triangular Quantum Billiard**

3a). Substituting the given wave functions in the Schrödinger equation yields

\[
-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi^{(j)}_{m,n}(x,y) = E_{m,n} \psi^{(j)}_{m,n}(x,y), \quad \text{for} \ j = 1, 2
\]

with \( E_{m,n} = \frac{4}{3}(m^2 + n^2 - mn) \left( \frac{2\pi}{\sqrt{3}L} \right)^2 \)

In terms of \( \rho_2 \) and \( \rho_3 \) the wavefunction \( \psi^{(2)}_{m,n}(x,y) \) can be expressed as

\[
\psi^{(2)}_{m,n}(x,y) = \sin[(2m - n) \frac{2\pi}{\sqrt{3}L} (\rho_2 - \rho_3)] \sin[n \frac{2\pi}{\sqrt{3}L} (\rho_2 + \rho_3)] \\
- \sin[(2n - m) \frac{2\pi}{\sqrt{3}L} (\rho_2 - \rho_3)] \sin[m \frac{2\pi}{\sqrt{3}L} (\rho_2 + \rho_3)] \\
+ \sin[-(m + n) \frac{2\pi}{\sqrt{3}L} (\rho_2 - \rho_3)] \sin[(m - n) \frac{2\pi}{\sqrt{3}L} (\rho_2 + \rho_3)]
\]

Putting \( \rho_2 = 0 \) we get,

\[
\psi^{(2)}_{m,n}(x,y) = \sin[(2m - n) \frac{2\pi}{\sqrt{3}L} (-\rho_3)] \sin[n \frac{2\pi}{\sqrt{3}L} (\rho_3)] \\
- \sin[(2n - m) \frac{2\pi}{\sqrt{3}L} (-\rho_3)] \sin[m \frac{2\pi}{\sqrt{3}L} (\rho_3)] \\
+ \sin[-(m + n) \frac{2\pi}{\sqrt{3}L} (-\rho_3)] \sin[(m - n) \frac{2\pi}{\sqrt{3}L} (\rho_3)]
\]

On simplification this gives 0. This implies that the wavefunction vanishes at the edge of the triangle defined by \( \rho_2 = 0 \). Proceeding exactly similarly it can be shown that both the wavefunctions vanish at all the sides of the triangle.

3b). The plots for \( \psi^{(1)}_{2,1}(x,y) \) and \( \psi^{(2)}_{3,1}(x,y) \) are shown below.
Figure 3: $\psi_{2,1}^{(1)}(x,y)$

Figure 4: $\psi_{3,1}^{(2)}(x,y)$
3c). Symmetries: $\psi^{(1)}_{m,n}(x,y)$ is symmetric under reflection about the x-axis while $\psi^{(2)}_{m,n}(x,y)$ is antisymmetric. Both the wavefunctions remain unchanged under rotation by $2\pi/3$ around the origin.

The path of a particle in an equilateral triangle can be considered to be lying in a 3D domain of phase space whose co-ordinates are the position $q = (x,y)$ and the path direction $\theta$. The path lies in a sequence of replicas of the triangle (sheets) situated at different values of $\theta$. The sheets are obtained by the reflection of the triangle along its edges. Reflection at a boundary corresponds to jumping between 2 sheets in $q-$, $\theta$-space. The six sheets form a hexagon. A path in this triangle is represented in this hexagon as a straight line with constant direction. The actions corresponding to the three paths parallel to the 3sides of triangle are

$$I_1 = \frac{3p_x}{4\pi} + \frac{\sqrt{3}p_y}{4\pi}$$

$$I_2 = \frac{3p_x}{4\pi} + \frac{\sqrt{3}p_y}{4\pi}$$

$$I_3 = \frac{\sqrt{3}p_y}{2\pi}$$

Quantization of the actions give the integers $m$ and $n$. 3d). As we found in part (a) the stationary states energies are given by

$$E_{m,n} = \frac{\hbar^2 x^2}{2m} \frac{4/3(2m^2 + n^2 - mn)}{(2\pi \sqrt{3L})^2}$$

Problem 4: Tunnelling through a delta barrier

4a). The Schrodinger eqn. is given by

$$-\frac{\hbar^2}{2m} \frac{d^2\phi_k(x)}{dx^2} + U(x)\phi_k(x) = E_k\phi_k(x)$$

where $U(x) = U_0\delta(x)$ and $E_k = \frac{\hbar^2 k^2}{2m}$

Integrating the solution from $-\epsilon$ to $+\epsilon$, we get

$$-\frac{\hbar^2}{2m} [\phi_k(\epsilon) - \phi_k(-\epsilon)] + U_0\phi_k(0) = E_k \int_{-\epsilon}^{\epsilon} \phi_k(x)dx \approx 2\epsilon E_k\phi_k(0)$$

Taking the limit $\epsilon \to 0$, we have
\[-\frac{\hbar^2}{2m} \lim_{\epsilon \to 0} [\phi_k'(\epsilon) - \phi_k'(-\epsilon)] + U_0 \phi_k(0) = 0\]

\[\lim_{\epsilon \to 0} [\phi_k'(\epsilon) - \phi_k'(-\epsilon)] = \frac{2mU_0}{\hbar^2} \phi_k(0)\]

4b. The wave-function of particles impinging from the left is given by
\[\phi_k(x) = Ae^{ikx}, \quad k^2 = \frac{2mE}{\hbar^2}\]

After incidence on the potential, the transmitted and reflected waves are given by
\[\phi_k(x) = Ae^{ikx} + Be^{-ikx} \text{ for } (x < 0)\]
\[\phi_k(x) = Ce^{ikx} \text{ for } (x > 0)\]

Continuity of the wavefunction and discontinuity of the derivative of the wavefunction at \(x = 0\) give
\[A + B = C\]
\[ik(C - A + B) = fC\]
\[f = \frac{2m}{\hbar^2} U_0\]

This gives,
\[B = -\frac{f}{f - 2ik} A\]
\[C = -\frac{2ik}{f - 2ik} A\]

B

The transmission coefficient is given by
\[T = \left| \frac{\langle j^> | j|m \rangle}{|\phi_k^{(trans)}|^2} \right|^2 = \frac{\hbar^4 k^2}{m^2 U_0^2 + \hbar^4 k^2} = \frac{\hbar^2 E}{\hbar^2 E + \frac{mU_0}{2}}\]
4c.) For a double delta function potential at \( x = 0 \) and \( x = a \), the wavefunctions in the three regions are given by

\[
\Psi_I = Ae^{ikx} + Be^{-ikx} \quad x < 0
\]
\[
\Psi_{II} = Ce^{ikx} + De^{-ikx} \quad 0 < x < a
\]
\[
\Psi_{III} = Ee^{ikx} \quad x > a
\]

The boundary conditions at \( X = 0 \) and \( X = a \) give

\[
A + B = C + D
\]
\[
iki(C - D - A + B) = f(C + D)
\]
\[
Ce^{ika} + De^{-ika} = Ee^{ika}
\]
\[
iki[Ee^{ika} - Ce^{ika} + De^{-ika}] = fEe^{ika}
\]

Solving the above equations we get for \( B \),

\[
B = -\frac{f^2 + f^2 e^{2ika} + 2ikf + 2ikf e^{2ika}}{-f^2 + 4k^2 + +4ikf + f^2 e^{2ika}} A
\]

The transmission coefficient is given by

\[
T = 1 - \frac{|B|^2}{|A|^2}
\]
\[
= 16k^4/[16k^4 + 8k^2 f^2 + 8k^2 f^2 \cos(2ka) + 2f^4 - 2f^4 \cos(2ka) + 8k f^3 \sin(2ka)]
\]
4d.)

Figure 5: T vs. k

4e). The wavefunction in the region $0 < x < a$ for the first 2 maxima of T is shown below.

Figure 6: $E = E^1$

Figure 7: $E = E^2$

4f.) The wavefunctions in the region $0 < x < a$ corresponding to the first two maxima of T corresponds to the levels $n = 1$ and $n = 2$ of a particle in a box.