

Solution to Problem Set 3

Physics 480 / Fall 1999

Prof. Klaus Schulten / Prepared by Pinaki Sengupta & Ioan Kosztin

Problem 1: Wave-Packet in 1-D Box

We start by defining suitable dimensionless parameters. We choose $a = 1$, $\hbar = 1$, $\tau = \frac{8ma^2}{\pi^2\hbar} = 1$. This implies $m = \pi^2/8$ and $E_n = n^2$. i) With the above choice of parameters, the range of E is $E = [2.5, 6.5]$ and σ 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 $\psi_0(x_0, t_0)$ 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. σ is taken as 0.2.

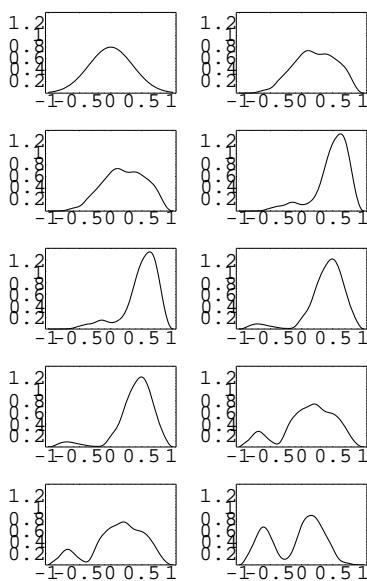


Figure 1: (i)

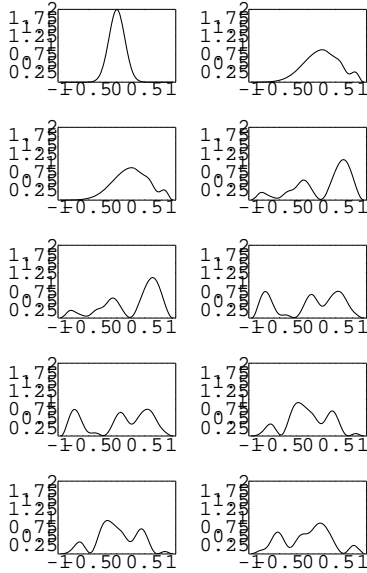


Figure 2: (ii)

Problem 2: Particle in 2-dimensional box

The stationary states wave function are determined by the time-independent Scrodinger 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 $\phi_{E_1}^{(e)}(x) = A_1 \cos k_1 x$ $\phi_{E_2}^{(e)}(y) = A_2 \cos k_2 y$

the odd solution $\phi_{E_1}^{(o)}(x) = A_1 \sin k_1 x$ $\phi_{E_2}^{(o)}(y) = A_2 \sin k_2 y$

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

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

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

The corresponding energy values are given by $E_n = \frac{\hbar^2 \pi^2}{8ma^2} n^2, n = 1, 2, 3, \dots$

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

$$\phi_n^{1(e)}(x) = A_{1n} \cos \frac{n\pi x}{2a}$$

$$\phi_n^{2(e)}(y) = A_{2n} \cos \frac{n\pi y}{2a}$$

$$\phi_n^{1(o)}(x) = A_{1n} \sin \frac{n\pi x}{2a}$$

$$\phi_n^{2(o)}(y) = A_{2n} \sin \frac{n\pi y}{2a}$$

Normalisation of the wave functions implies $A_{1n} = A_{2n} = \sqrt{\frac{1}{a}}$ Thus the complete wave functions are give by

$$\phi_{n_1, n_2}(x, y) = \frac{1}{a} \begin{cases} \cos \frac{n_1 \pi x}{2a} \cos \frac{n_2 \pi y}{2a} & \text{for } n_1, n_2 = 1, 3, 5 \dots \\ \sin \frac{n_1 \pi x}{2a} \sin \frac{n_2 \pi y}{2a} & \text{for } n_1, n_2 = 2, 4, 6 \dots \end{cases}$$

with energy

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

Symmetries

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

1. Rotation by π 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.

n_1, n_2	$E/\frac{\hbar^2\pi^2}{8ma^2}$	degeneracy
1,1	2	single
1,2	5	two-fold
2,2	8	single
1,3	10	two-fold
2,3	13	two-fold

Problem 3: Triangular Quantum Billiard

3a). Substituting the given wave functions in the Schrodinger equation yeilds

$$-\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2)\psi_{m,n}^{(j)}(x, y) = E_{m,n}\psi_{m,n}^{(j)}(x, y), \quad \text{for } j = 1, 2$$

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

In terms of ρ_2 and ρ_3 the wavefunction $\psi_{m,n}^{(2)}(x, y)$ can be expressed as

$$\begin{aligned} \psi_{m,n}^{(2)}(x, y) &= \sin\left[(2m - n)\frac{2\pi}{3\sqrt{3}L}(\rho_2 - \rho_3)\right] \sin\left[n\frac{2\pi}{\sqrt{3}L}(\rho_2 + \rho_3)\right] \\ &\quad - \sin\left[(2n - m)\frac{2\pi}{3\sqrt{3}L}(\rho_2 - \rho_3)\right] \sin\left[m\frac{2\pi}{\sqrt{3}L}(\rho_2 + \rho_3)\right] \\ &\quad + \sin\left[-(m + n)\frac{2\pi}{3\sqrt{3}L}(\rho_2 - \rho_3)\right] \sin\left[(m - n)\frac{2\pi}{\sqrt{3}L}(\rho_2 + \rho_3)\right] \end{aligned}$$

Putting $\rho_2 = 0$ we get,

$$\begin{aligned} \psi_{m,n}^{(2)}(x, y) &= \sin\left[(2m - n)\frac{2\pi}{3\sqrt{3}L}(-\rho_3)\right] \sin\left[n\frac{2\pi}{\sqrt{3}L}(\rho_3)\right] \\ &\quad - \sin\left[(2n - m)\frac{2\pi}{3\sqrt{3}L}(-\rho_3)\right] \sin\left[m\frac{2\pi}{\sqrt{3}L}(\rho_3)\right] \\ &\quad + \sin\left[-(m + n)\frac{2\pi}{3\sqrt{3}L}(-\rho_3)\right] \sin\left[(m - n)\frac{2\pi}{\sqrt{3}L}(\rho_3)\right] \end{aligned}$$

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 $\psi_{2,1}^{(1)}(x, y)$ and $\psi_{3,1}^{(2)}(x, y)$ are shown below.

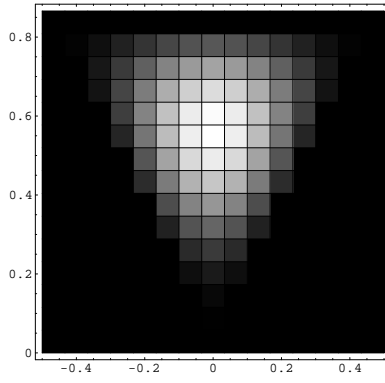


Figure 3: $\psi_{2,1}^{(1)}(x, y)$

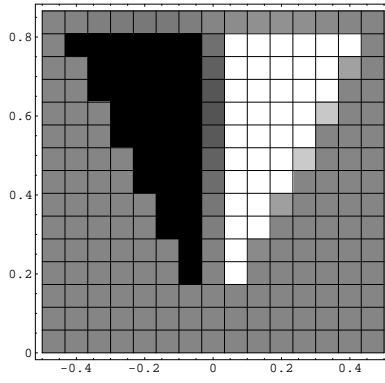


Figure 4: $\psi_{3,1}^{(2)}(x, y)$

3c.) Symmetries: $\psi_{m,n}^{(1)}(x, y)$ is symmetric under reflection about the x-axis while $\psi_{m,n}^{(2)}(x, y)$ 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 $q^\rightarrow = (x, y)$ and the path direction θ . The path lies in a sequence of replicas of the triangle (sheets) situated at different values of θ . 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^\rightarrow, θ 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 3 sides 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

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

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

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

$$\cong 2\epsilon E_k \phi_k(0)$$

Taking the limit $\epsilon \rightarrow 0$, we have

$$-\frac{\hbar^2}{2m} \lim_{\epsilon \rightarrow 0} [\phi'_k(\epsilon) - \phi'_k(-\epsilon)] + U_0 \phi_k(0) = 0$$

$$\lim_{\epsilon \rightarrow 0} [\phi'_k(\epsilon) - \phi'_k(-\epsilon)] = \frac{2mU_0}{\hbar^2} \phi_k(0)$$

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

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

$$\begin{aligned} T &= \left| \frac{j_{>}}{j_{in}} \right| \\ &= \frac{|\phi_k^{trans}|^2}{|\phi_k^{in}|^2} \\ &= \frac{\hbar^4 k^2}{m^2 U_0^2 + \hbar^4 k^2} \\ &= \frac{\hbar^2 E}{\hbar^2 E + \frac{mU_0}{2}} \end{aligned}$$

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

$$A + B = C + D$$

$$ik(C - D - A + B) = f(C + D)$$

$$Ce^{ika} + De^{-ika} = Ee^{ika}$$

$$ik[Ce^{ika} - Ee^{ika} + De^{-ika}] = fEe^{ika}$$

Solving the above equations we get for B,

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

The transmission coefficient is given by

$$\begin{aligned} T &= 1 - \frac{|B|^2}{|A|^2} \\ &= 16k^4 / \{16k^4 + 8k^2f^2 + 8k^2f^2\cos(2ka) + 2f^4 - 2f^4\cos(2ka) + 8kf^3\sin(2ka)\} \end{aligned}$$

4d.)

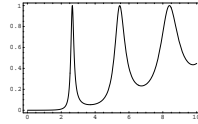


Figure 5: T vs. k

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

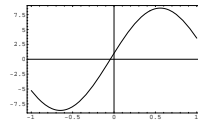


Figure 6: $E = E^1$

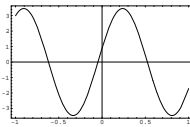


Figure 7: $E = E^2$

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