1. A square well potential is given by $V(x) = -V_0$ if $|x| < a$, and 0 otherwise. The energy eigenfunctions (even boundstates) are given by

$$\phi_n(x) = \begin{cases} A\cos\left(\xi_n \frac{x}{a}\right) & |x| < a \\ F\exp\left(-\eta_n \frac{|x|}{a}\right) & \text{otherwise} \end{cases}$$

where η_n and ξ_n are positive numbers.

   (a) Find F in terms of A.
   (b) Find A by normalizing the wave function. (Express A in terms of a, ξ_n and, η_n).
   (c) Find the expression for the probability that the particle will be found outside the well if it is in state ϕ_n at a given instant.
   (d) Do the same excercise for odd boundstates.

2. Set $\hbar = m = a = 1$ and $V_0 = 50$ in the square well potential, given in problem 1. Then $\gamma^2 = 2V_0$, $\xi^2 = \alpha^2 = 2(V_0 + E)$ and $\eta^2 = \beta^2 = -2E$.

   (a) Estimate the number of boundstates.
   (b) Solve the equations

$$\xi\tan\xi = \sqrt{\gamma^2 - \xi^2}$$

   and

$$-\xi\cot\xi = \sqrt{\gamma^2 - \xi^2}$$

   numerically by any method (one method is given below) to obtain the energy spectrum.
   (c) Find the normalization constants for each bound state.
   (d) Find the probability that particle is found outside the well for the ground state and the highest energy state.

3. Consider a potential given by

$$V(x) = \begin{cases} \infty & x < 0 \\ -V_0 & 0 < x < a \\ 0 & x > a \end{cases}$$

Find out the condition determining the energy eigenvalues of the bound states of this potential.

4. If a wavefunction is given by $\psi(x) = c\,f(x)$, where c is a constant (may be complex) and f is a real-valued function, show that the probability current density vanishes everywhere.

5. Consider a wavepacket given by

$$\Psi(x, t = 0) = A\exp\left(-\frac{(x - x_0)^2}{2\sigma^2}\right)\exp\left(i\frac{p_0 x}{\hbar}\right).$$

Find the probability current density.

6. The potential energy is given by

$$V(x) = \begin{cases} V_0 & x > 0 \\ 0 & x < 0. \end{cases}$$

Find the transmission and reflection coefficients assuming a plane wave incident from the left side with energy $E > V_0$.

7. Determine the transmission coefficient for a rectangular barrier with the potential given by

$$V(x) = \begin{cases} +V_0 & \text{if } |x| < a \\ 0 & \text{otherwise} \end{cases}$$

where V_0 is a positive constant. Treat the three cases, $E < V_0$, $E = V_0$, and $E > V_0$ separately.

8. Find the scattering matrix for the rectangular barrier given in problem 7 assuming $E > V_0$.

Solution 2:

Fixed Point Iterative method: Transform the first equation to

$$\xi = g(\xi) = (n-1)\frac{\pi}{2} + \tan^{-1}\left(\frac{\sqrt{\gamma^2 - \xi^2}}{\xi}\right).$$

Here $n = 1, 3, \ldots$. $g(\xi)$ is called iterating function. Now use iterative method, that is

$$\xi^{(k+1)} = g(\xi^{(k)}) = (n-1)\frac{\pi}{2} + \tan^{-1}\left(\frac{\sqrt{\gamma^2 - \left(\xi^{(k)}\right)^2}}{\xi^{(k)}}\right).$$

You must choose the initial guess, that is, $\xi^{(0)}$. Choose a value closer to the solutions. There is a theorem that claims that $\xi^{(k)}$ converges to a root for $k \to \infty$. To get an accuracy of two or three digits, you may have to go upto $k = 4$ or 5. Do this on your calculator. Here is an example, for $n = 1$, let $\xi^{(0)} = 1$, then $\xi^{(1)} = 1.4706$, $\xi^{(2)} = 1.4232$, $\xi^{(3)} = 1.4280$, $\xi^{(4)} = 1.4276$ and $\xi^{(5)} = 1.4275$. Here is complete table.

n	ξ_n	E_n	A_n	$P(\|x\| > a)$ %
1	1.4275	-48.9811	0.9530	0.19
2	2.8523	-45.9321	0.9516	0.77
3	4.2711	-40.8789	0.9489	1.82
4	5.6792	-33.8733	0.9443	3.49
5	7.0689	-25.0154	0.9360	6.19
6	8.4232	-14.5249	0.9148	11.10
7	9.6789	-3.1596	0.8458	26.66

Solutions:

1. Given

$$\phi_n(x) = \begin{cases} A\cos\left(\xi_n \frac{x}{a}\right) & |x| < a \\ F\exp\left(-\eta_n \frac{|x|}{a}\right) & \text{otherwise} \end{cases}$$

(a) At $x = a$, ϕ_n must be continuous, hence

$$\begin{aligned} A\cos(\xi_n) &= F\exp(-\eta_n) \\ \Longrightarrow F &= A\frac{\cos(\xi_n)}{\exp(-\eta_n)} \end{aligned}$$

(b) Square of the norm of ϕ_n is

$$\begin{aligned} \int_{-\infty}^{\infty} |\phi_n(x)|^2\,dx &= 2\int_0^{\infty} |\phi_n(x)|^2\,dx \\ &= 2\int_0^a |A|^2\cos^2\left(\xi_n\frac{x}{a}\right) + 2\int_a^{\infty} |F|^2\exp\left(-2\eta_n\frac{x}{a}\right)dx \\ &= |A|^2\left[a\left(1 + \frac{\sin(2\xi_n)}{2\xi_n} + \frac{\cos^2\xi_n}{\eta_n}\right)\right] \end{aligned}$$

Thus,

$$A = \left[a\left(1 + \frac{\sin(2\xi_n)}{2\xi_n} + \frac{\cos^2\xi_n}{\eta_n}\right)\right]^{-1/2}$$

(c) Probability that the particle is found outside the well is

$$\begin{aligned} P\left(\left|\hat{X}\right| > a\right) &= 2\int_a^{\infty} |F|^2\exp\left(-2\eta_n\frac{x}{a}\right)dx. \\ &= \frac{A^2 a}{\eta_n}\cos^2(\xi_n) \end{aligned}$$

(d) For odd states,

$$\phi_n(x) = \begin{cases} A\sin\left(\xi_n\frac{x}{a}\right) & |x| < a \\ F\exp\left(-\eta_n\frac{|x|}{a}\right) & x > a \\ -F\exp\left(-\eta_n\frac{|x|}{a}\right) & x < -a \end{cases}$$

Follow simillar procedure to obtain

$$A = \left[a\left(1 - \frac{\sin(2\xi_n)}{2\xi_n} + \frac{\sin^2\xi_n}{\eta_n}\right)\right]^{-1/2}$$

and

$$P\left(\left|\hat{X}\right| > a\right) = \frac{A^2 a}{\eta_n}\sin^2(\xi_n)$$

2. Given above.

3. Boundary conditions for the wave function:

   (a) At $x = a$, the wave function and its first derivative must be continuous.
   (b) At $x = 0$, the wave function must vanish.

   For bound states, energy eigenvalue, $E < 0$.General solution in Region I ($x \in [0, a]$),

   $$\phi_I = A\sin(\alpha x) + B\cos(\alpha x)$$

   and in Region 2 ($x > a$),

   $$\phi_{II} = Ce^{\beta x} + De^{-\beta x},$$

   where $\beta = \sqrt{2mE}/\hbar$ and $\alpha = \sqrt{2m(E + V_0)}/\hbar$. Applying boundary condition (b), we get $B = 0$. And applying boundary condition (a), we get

   $$\eta = -\xi\cot\xi.$$

   This is exactly same as in case of the odd eigen-states of a square well potential. We could have arrived at this conclusion just by guessing.

4. Given: $\psi(x) = cf(x)$, where f is a real function of x and c may be a complex constant.

$$\begin{aligned} J(x) &= \frac{\hbar}{2mi}\left[\psi^* \frac{\partial}{\partial x}\psi - \psi \frac{\partial}{\partial x}\psi^*\right] \\ &= \frac{\hbar}{2mi}|c|^2\left[f\frac{\partial}{\partial x}f - f\frac{\partial}{\partial x}f\right] = 0. \end{aligned}$$

5. Probability current density is

$$\begin{aligned} J(x) &= \frac{\hbar}{2mi}\left[\psi^* \frac{\partial}{\partial x}\psi - \psi \frac{\partial}{\partial x}\psi^*\right] \\ &= \frac{\hbar}{2mi}|A|^2 \exp\left(-\frac{(x-x_0)^2}{\sigma^2}\right)\left[\left(-\frac{(x-x_0)}{\sigma^2} + i\frac{p_0}{\hbar}\right) - \left(-\frac{(x-x_0)}{\sigma^2} - i\frac{p_0}{\hbar}\right)\right] \\ &= \frac{p_0}{m}|A|^2 \exp\left(-\frac{(x-x_0)^2}{\sigma^2}\right) \end{aligned}$$

6. Assuming $E > V_0$, the solution to the Schrodinger equation is

$$\psi(x) = \begin{cases} Ae^{i\alpha x} + Be^{-i\alpha x} & x < 0 \\ Ce^{i\beta x} & x > 0, \end{cases}$$

where $\alpha = \sqrt{2mE}/\hbar$, and $\beta = \sqrt{2m(E-V_0)}/\hbar$. Applying BC at $x = 0$, we get

$$\begin{aligned} A + B &= C \\ A - B &= \frac{\beta}{\alpha}C \end{aligned}$$

Thus

$$\frac{C}{A} = \frac{2\alpha}{\alpha+\beta}$$

and

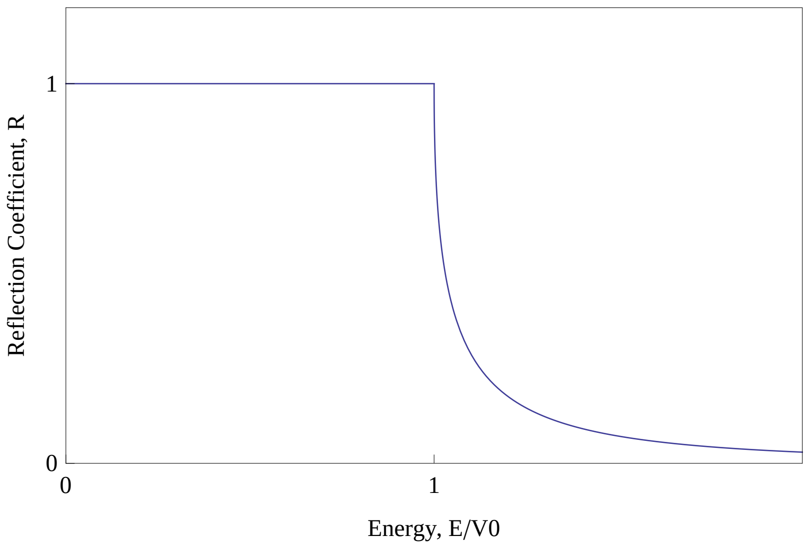
$$\frac{B}{A} = \frac{\beta-\alpha}{\alpha+\beta}$$

The transmission coefficient is

$$T = \frac{J_t}{J_i} = \frac{\beta}{\alpha}\left|\frac{C}{A}\right|^2 = \frac{2\alpha\beta}{(\alpha+\beta)^2}$$

and

$$\begin{aligned} R &= \left|\frac{B}{A}\right|^2 = \frac{(\alpha-\beta)^2}{(\alpha+\beta)^2} = \frac{\left(\sqrt{E}-\sqrt{E-V_0}\right)^2}{\left(\sqrt{E}+\sqrt{E-V_0}\right)^2} \\ &= 1 \qquad \frac{E}{V_0} = 1 \\ &\to 0 \qquad \frac{E}{V_0} \gg 1 \end{aligned}$$



7. The transmission coefficient for rectangular barrier is given by

$$\begin{aligned} T &= \left[1 + \frac{V_0^2 \sinh^2(2\beta a)}{4E(V_0 - E)}\right]^{-1} \qquad E < V_0 \\ &\rightarrow \frac{1}{1 + 2mV_0 a^2/\hbar^2} \quad \text{as } E \rightarrow V_0 \\ &= \left[1 + \frac{V_0^2 \sin^2(2\beta a)}{4E(V_0 - E)}\right]^{-1} \qquad E > V_0 \end{aligned}$$

where, $\beta = \sqrt{2m(E - V_0)}/\hbar$.

8. The solution of the SE is

$$\psi(x) = \begin{cases} Ae^{i\alpha x} + Be^{-i\alpha x} & x < -a \\ Ce^{i\beta x} + De^{-i\beta x} & -a < x < a, \\ Ee^{i\alpha x} + Ee^{-i\alpha x} & a < x \end{cases}$$

where $\alpha = \sqrt{2mE}/\hbar$, and $\beta = \sqrt{2m(E - V_0)}/\hbar$. Applying BC at $x = -a$, we get

$$\begin{aligned} \begin{bmatrix} \bar{q} & q \\ \beta\bar{q} & -\beta q \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} &= \begin{bmatrix} \bar{p} & p \\ \alpha\bar{p} & -\alpha p \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} \\ \begin{bmatrix} C \\ D \end{bmatrix} &= \frac{1}{2} \begin{bmatrix} q & \frac{1}{\beta} q \\ \bar{q} & -\frac{1}{\beta}\bar{q} \end{bmatrix} \begin{bmatrix} \bar{p} & p \\ \alpha\bar{p} & -\alpha p \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} \end{aligned}$$

Applying BC at $x = a$, we get

$$\begin{aligned} \begin{bmatrix} p & \bar{p} \\ \alpha p & -\alpha\bar{p} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} &= \begin{bmatrix} q & \bar{q} \\ \beta q & -\beta\bar{q} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} \\ \begin{bmatrix} p & \bar{p} \\ \alpha p & -\alpha\bar{p} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} &= \frac{1}{2} \begin{bmatrix} q & \bar{q} \\ \beta q & -\beta\bar{q} \end{bmatrix} \begin{bmatrix} q & \frac{1}{\beta} q \\ \bar{q} & -\frac{1}{\beta}\bar{q} \end{bmatrix} \begin{bmatrix} \bar{p} & p \\ \alpha\bar{p} & -\alpha p \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} \\ \begin{bmatrix} p & \bar{p} \\ \alpha p & -\alpha\bar{p} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} &= \begin{bmatrix} \cos(2\beta a) & \frac{i}{\beta}\sin(2\beta a) \\ i\beta\sin(2\beta a) & \cos(2\beta a) \end{bmatrix} \begin{bmatrix} \bar{p} & p \\ \alpha\bar{p} & -\alpha p \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} \end{aligned}$$

Without substituting for p, we can simplify this to

$$\begin{aligned} B &= \frac{\bar{p}^2 \left(\left(\alpha^2 - \beta^2\right)\sin(2\beta a)\, A + 2i\alpha\beta F\right)}{2i\alpha\beta\cos(2\beta a) + (\alpha^2 + \beta^2)\sin(2\beta a)} \\ E &= \frac{\bar{p}^2 \left(2i\alpha\beta A + \left(\alpha^2 - \beta^2\right)\sin(2\beta a)\, F\right)}{2i\alpha\beta\cos(2\beta a) + (\alpha^2 + \beta^2)\sin(2\beta a)} \end{aligned}$$

Now we can write down the scattering matrix. The transmission coefficient can be found by setting $F = 0$. Compare with solution of 7.