Solution to MIT 8.05 Problem Set 1 (Problems 3 & 4)

Problem 3: Three Delta Functions

Consider a particle of mass m moving in a potential consisting of three attractive delta functions:

$$V(x) = -V_0 a\left[\delta(x+a) + \delta(x) + \delta(x-a)\right] \tag{1}$$

where $V_0 > 0$ and $a > 0$.

(a) Discontinuities in the first derivative

The Schrödinger equation is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{2}$$

Integrating this equation from $x_i - \epsilon$ to $x_i + \epsilon$ around a delta function location x_i (where $x_i \in \{-a, 0, a\}$):

$$-\frac{\hbar^2}{2m}\int_{x_i-\epsilon}^{x_i+\epsilon}\frac{d^2\psi}{dx^2}dx + \int_{x_i-\epsilon}^{x_i+\epsilon}V(x)\psi(x)dx = \int_{x_i-\epsilon}^{x_i+\epsilon}E\psi(x)dx \tag{3}$$

Taking the limit as $\epsilon \to 0$, the RHS vanishes because ψ is continuous. The potential term contributes due to the delta function $\delta(x - x_i)$ with weight $-V_0 a$.

$$-\frac{\hbar^2}{2m}\left(\psi'(x_i^+) - \psi'(x_i^-)\right) - V_0 a\psi(x_i) = 0 \tag{4}$$

Thus, the discontinuity in the first derivative at any of the three points is:

$$\Delta\psi'(x_i) = \psi'(x_i^+) - \psi'(x_i^-) = -\frac{2mV_0 a}{\hbar^2}\psi(x_i) \tag{5}$$

Let us define a dimensionless parameter $\lambda \equiv \frac{mV_0a^2}{\hbar^2}$. Then:

$$\Delta\psi'(x_i) = -\frac{2\lambda}{a}\psi(x_i) \tag{6}$$

(b) Nodes in bound state wavefunctions

For bound states ($E < 0$), let $\kappa = \sqrt{-2mE}/\hbar$.

- **Region $x > a$:** The potential is zero. The solution must decay at infinity: $\psi(x) \sim e^{-\kappa x}$. This is a monotonic function and **cannot have nodes**.
- **Region $0 < x < a$:** The particle behaves like a free particle. The solution is a linear combination of $e^{\kappa x}$ and $e^{-\kappa x}$ (or sinh and cosh). These functions **can have nodes**.
- **At $x = a$:** Can $\psi(a) = 0$? If $\psi(a) = 0$, the discontinuity condition from part (a) implies $\psi'(a^+) - \psi'(a^-) \propto \psi(a) = 0$, so the derivative is continuous. Since $\psi(x) = Ae^{-\kappa x}$ for $x > a$, if $\psi(a) = 0$, then A must be 0, leading to the trivial solution $\psi(x) \equiv 0$ everywhere. Thus, **no node can exist exactly at the well $x = a$.**
- **At $x = 0$:** For antisymmetric states, $\psi(-x) = -\psi(x)$, which implies $\psi(0) = 0$. Thus, **a node can exist at $x = 0$.**

(c) Limit of large separation (or large V_0)

If the wells are very deep or far apart, the tunneling between them is weak.

- Since there are three attractive wells, we expect **three bound states**.
- The wavefunctions will be linear combinations of the single-well ground states.
- By the node theorem (ground state has 0 nodes, n-th excited state has n nodes):
  1. **Ground State:** Symmetric, no nodes (peaks at all three wells). $\psi \sim (+,+,+)$.
  2. **First Excited State:** Antisymmetric, one node at $x=0$. $\psi \sim (+,0,-)$.
  3. **Second Excited State:** Symmetric, two nodes (between the wells). $\psi \sim (+,-,+)$.

(d) Lowest Energy Antisymmetric Bound State

For the antisymmetric state, $\psi(x) = -\psi(-x)$, so $\psi(0) = 0$. The delta function at $x = 0$ has no effect because $V(x)\psi(x) \propto \delta(x)\psi(x) = 0$. The problem reduces to a particle in the region $x > 0$ with an infinite wall at $x = 0$ and a delta well at $x = a$.

Ansatz:

$$0 < x < a: \quad \psi(x) = A\sinh(\kappa x) \quad \text{(ensures } \psi(0) = 0\text{)} \tag{7}$$

$$x > a: \quad \psi(x) = Be^{-\kappa(x-a)} \quad \text{(ensures decay at } \infty\text{)} \tag{8}$$

Matching at $x = a$: 1. Continuity of ψ:

$$A\sinh(\kappa a) = B \tag{9}$$

2. Discontinuity of ψ':

$$\psi'(a^+) - \psi'(a^-) = -\frac{2\lambda}{a}\psi(a) \tag{10}$$

Differentiating the ansatz:

$$-\kappa B - \kappa A\cosh(\kappa a) = -\frac{2\lambda}{a}B \tag{11}$$

Substitute $B = A\sinh(\kappa a)$:

$$-\kappa A\sinh(\kappa a) - \kappa A\cosh(\kappa a) = -\frac{2\lambda}{a}A\sinh(\kappa a) \tag{12}$$

Assuming $A \neq 0$, divide by $-A$ and multiply by a:

$$\kappa a(\sinh(\kappa a) + \cosh(\kappa a)) = 2\lambda\sinh(\kappa a) \tag{13}$$

Using $e^{\kappa a} = \sinh + \cosh$:

$$\kappa a e^{\kappa a} = \lambda(e^{\kappa a} - e^{-\kappa a}) \tag{14}$$

Divide by $e^{\kappa a}$:

$$\kappa a = \lambda(1 - e^{-2\kappa a}) \tag{15}$$

This is the transcendental equation for the energy.

Condition for existence: A bound state exists if a solution for $\kappa > 0$ exists. The critical case is when the binding energy goes to zero, i.e., $\kappa \to 0$. Expand the RHS for small κa:

$$\text{RHS} \approx \lambda(1 - (1 - 2\kappa a)) = 2\lambda\kappa a \tag{16}$$

The equation becomes $\kappa a = 2\lambda\kappa a$. For a non-trivial solution, the slope of the RHS must be greater than the slope of the LHS at the origin (or exactly equal at the limit):

$$2\lambda > 1 \implies \lambda > \frac{1}{2} \tag{17}$$

Recalling $\lambda = \frac{mV_0a^2}{\hbar^2}$, the condition for the existence of an antisymmetric bound state is:

$$V_0 > \frac{\hbar^2}{2ma^2} \tag{18}$$

Problem 4: Estimates on the Finite Square Well

Consider a finite square well potential:

$$V(x) = \begin{cases} -V_0 & |x| \leq a \\ 0 & |x| > a \end{cases} \tag{19}$$

The standard dimensionless parameter describing the "strength" of the well is:

$$z_0 = \frac{a}{\hbar}\sqrt{2mV_0} \tag{20}$$

The number of bound states depends on the intersections of a circle of radius z_0 with the curves $\tan(z)$ (for even parity states) and $-\cot(z)$ (for odd parity states) in the first quadrant of the (k, κ) plane, or more simply, solving the transcendental equations:

$$\tan z = \sqrt{(z_0/z)^2 - 1} \quad \text{(Even)} \tag{21}$$

$$-\cot z = \sqrt{(z_0/z)^2 - 1} \quad \text{(Odd)} \tag{22}$$

Estimate of the number of states

New bound states appear every time z_0 crosses a multiple of $\pi/2$.

- $0 < z_0 < \pi/2$: Only 1 state (even).
- $\pi/2 < z_0 < \pi$: 2 states (1 even, 1 odd).
- $\pi < z_0 < 3\pi/2$: 3 states.

Generally, the number of bound states N is given exactly by:

$$N = \left\lfloor \frac{2z_0}{\pi} \right\rfloor + 1 \tag{23}$$

where $\lfloor x \rfloor$ denotes the floor function (the greatest integer less than or equal to x).

For a very deep well ($z_0 \gg 1$), we can approximate this simply as:

$$N \approx \frac{2z_0}{\pi} \tag{24}$$

Substituting the definition of z_0:

$$N \approx \frac{2}{\pi}\frac{a}{\hbar}\sqrt{2mV_0} = \frac{2a}{\pi\hbar}\sqrt{2mV_0} \tag{25}$$

This confirms that the number of bound states increases linearly with the width a and with the square root of the depth V_0.