Finite Potential Well

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Finite Square Well

The finite square well is a potential energy function that is defined piecewise as follows:

$$V(x) = \begin{cases} -V_0 & \text{if } -a \leq x \leq a, \\ 0 & \text{otherwise.} \end{cases}$$

The mass of ^{87}Rb is $m = 1.443 \times 10^{-25}$ kg.

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

The condition for having three bound states corresponds to z_0 lying within a range that supports exactly three bound energy levels. The range is given by the following inequality:

$$\pi < z_0 < \frac{3\pi}{2}$$

Let choose $a = 1nm = 1 \cdot 10^{-9}$ m and $z_0 = 4$. We can calculate the value of V_0 that satisfies the condition for having three bound states. We can reagrange the equation to solve for V_0:

$$|V_0| = \frac{(z_0)^2\hbar^2}{2ma^2} = \frac{(4)^2\,(1.055 \cdot 10^{-34})^2}{2(1.443 \cdot 10^{-25})(1 \cdot 10^{-9})^2} \approx 6.1706 \cdot 10^{-25} J \approx 3.8514 \cdot 10^{-6} eV$$

Where a is half-width of the Well.

In the region of $x < -a$, the potential is zero, we have the Shrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \text{ or } \frac{d^2\psi}{dx^2} = \kappa^2\psi \tag{1}$$

Where: $\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$

$$\psi_1 = Ae^{\kappa x} \tag{2}$$

In the region of $-a \leq x \leq a$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi, \text{ or } \frac{d^2\psi}{dx^2} = -l^2\psi \tag{3}$$

Where: $l \equiv \frac{\sqrt{2m(V_0+E)}}{\hbar}$

$$\psi_2 = B\sin(lx) + C\cos(lx) \tag{4}$$

In the region of $x > a$:

$$E\psi = -\frac{\hbar}{2m}\frac{d^2\psi}{dx^2} \text{ or } \frac{d^2\psi}{dx^2} = \kappa^2\psi \tag{5}$$

$$\psi_3 = De^{-\kappa x} \tag{6}$$

For the even bound states:

$$\psi(x) = \begin{cases} Ae^{\kappa x} & \text{if } x < -a, \\ C\cos(lx) & \text{if } -a \leq x \leq a, \\ De^{-\kappa x} & \text{if } x > a. \end{cases} \tag{7}$$

It's transcendental equation is $\tan(z) = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ where $z = la$

Plug in the constants, we have:

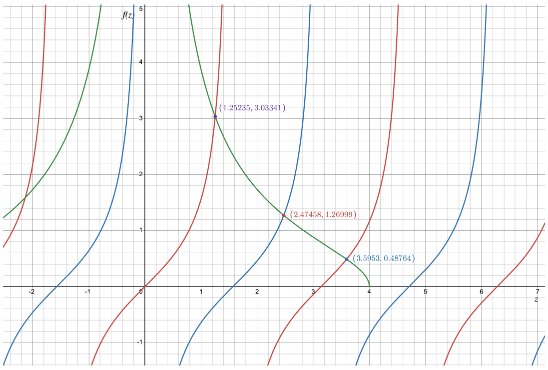
$$z = la = \frac{\sqrt{2m(V_0 + E)}}{\hbar} a = \frac{\sqrt{2(1.443 \cdot 10^{-25})(6.1706 \cdot 10^{-25} J + E)}}{1.055 \cdot 10^{-34} J} \cdot 10^{-9} \tag{8}$$

For the odd bound states:

$$\psi(x) = \begin{cases} Ae^{\kappa x} & \text{if } x < -a, \\ B\sin(lx) & \text{if } -a \leq x \leq a, \\ De^{-\kappa x} & \text{if } x > a. \end{cases} \tag{9}$$

It's transcendental equation is $-\cot(z) = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$

The graph of even and odd bound states are shown below:



(a) Even and Odd Bound States

The red line is the function of $f(z) = \tan(z)$ and the blue line is the function of $g(z) = -\cot(z)$, the green line is the function of $h(z) = \sqrt{\left(\frac{4}{z}\right)^2 - 1}$ at $z_0 = 4$. We can see there are 3 intersections at $z_0 = 1.25235\,(\text{even}), z_1 = 2.47458\,(\text{odd}), z_2 = 3.5953\,(\text{even})$. Plug in the value of z_n for equation (8). We can get the value of E_n.

$$E_0 \approx -5.57113 \cdot 10^{-25}\,(J), l_0 \approx 1.2523 \cdot 10^9, \kappa_0 \approx 3.8 \cdot 10^9$$
$$E_1 \approx -3.80897 \cdot 10^{-25}\,(J), l_1 \approx 2.47458 \cdot 10^9, \kappa_1 \approx 3.14 \cdot 10^9$$
$$E_2 \approx -1.18544 \cdot 10^{-25}\,(J), l_2 \approx 3.5953 \cdot 10^9, \kappa_2 \approx 1.75 \cdot 10^9$$

Now we normalize the wave function for the even bound states to find the value of A, C, D from equation (7). We have:

$$\begin{aligned}
1 = \int_{-\infty}^{\infty} |\psi(x)|^2 dx &= \int_{-\infty}^{-a} |Ae^{\kappa x}|^2 dx + \int_{-a}^{a} |C\cos(lx)|^2 dx + \int_{a}^{\infty} |De^{-\kappa x}|^2 dx \\
&= (A^2 + D^2) \int_a^{\infty} e^{-2kx} dx + 2C^2 \int_0^a \cos^2(lx) dx \\
&= (A^2 + D^2) \frac{e^{-2\kappa a}}{2\kappa} + 2C^2 \left(\frac{2al + \sin(2al)}{4l} \right) \\
&= (A^2 + D^2) \frac{e^{-2\kappa a}}{2\kappa} + C^2 \left(a + \frac{\sin(2al)}{2l} \right)
\end{aligned}$$

Since the wave equation is continous at $x = \pm a$, we have:

$$\begin{aligned}
Ae^{-ka} &= C\cos(-la) \text{ at } x = -a \\
\Rightarrow A &= e^{ka} C \cos(-la) \\
De^{-ka} &= C\cos(la) \text{ at } x = a \\
\Rightarrow D &= e^{ka} C \cos(la)
\end{aligned}$$

And we have $\cos(la) = \cos(-la)$, therefore $A = D$. Plug in the value of A, D to the normalization equation, we have:

$$\begin{aligned}
1 &= 2C^2 e^{2ka}\cos^2(la)\frac{e^{-2\kappa a}}{2\kappa} + C^2\left(a + \frac{\sin(2al)}{2l}\right) \\
&= C^2 e^{2ka}\cos^2(la)\frac{e^{-2\kappa a}}{\kappa} + C^2\left(a + \frac{\sin(2al)}{2l}\right) \\
&= C^2\left(\frac{\cos^2(la)}{k} + \frac{\sin(2al)}{2l} + a\right) = C^2\left(a + \frac{1}{k}\right) = 1 \\
&\Rightarrow C = \sqrt{\frac{1}{a + \frac{1}{k}}} \text{ and } A = D = \frac{e^{ak}\cos(la)}{\sqrt{a + \frac{1}{k}}}
\end{aligned}$$

Now for the odd bound states, we have:

$$\begin{aligned}
1 &= \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{-a} |Ae^{\kappa x}|^2 dx + \int_{-a}^{a} |B\sin(lx)|^2 dx + \int_{a}^{\infty} |De^{-\kappa x}|^2 dx \\
&= (A^2 + D^2)\int_a^{\infty} e^{-2kx}dx + 2B^2\int_0^a \sin^2(lx)dx \\
&= (A^2 + D^2)\frac{e^{-2\kappa a}}{2\kappa} + 2B^2\left(\frac{a}{2} - \frac{\sin(2al)}{4l}\right) \\
&= (A^2 + D^2)\frac{e^{-2\kappa a}}{2\kappa} + B^2\left(a - \frac{\sin(2al)}{2l}\right)
\end{aligned}$$

Since the wave equation is continous at $x = \pm a$, we have:

$$\begin{aligned}
Ae^{-ka} &= B\sin(-la) \text{ at } x = -a \\
\Rightarrow A &= e^{\kappa a}B\sin(-la) \\
De^{-ka} &= B\sin(la) \text{ at } x = a \\
\Rightarrow D &= e^{ka}B\sin(la)
\end{aligned}$$

Since $\sin(-la) = -\sin(la)$, we have $A = -D$. Plug in the value of A, D to the normalization equation, we have:

$$\begin{aligned}
1 &= \left[(-e^{ka}B\sin(la))^2 + (e^{ka}B\sin(la))^2\right]\frac{e^{-2\kappa a}}{2\kappa} + B^2\left(a - \frac{\sin(2al)}{2l}\right) \\
&= 2B^2 e^{2ka}\sin^2(la)\frac{e^{-2\kappa a}}{2\kappa} + B^2\left(a - \frac{\sin(2al)}{2l}\right) \\
&= B^2\left(\frac{\sin^2(la)}{k} + a - \frac{\sin(2al)}{2l}\right)
\end{aligned}$$

For this one if we have $-\kappa = l\cot(la)$

$$
\begin{aligned}
1 &= B^2\left(\frac{\sin^2(la)}{-l\cot(la)} - \frac{2\sin(la)cos(la)}{2l} + a\right) \\
&= B^2\left(\frac{\sin^2(la)}{-l\frac{\cos(la)}{\sin(la)}} - \frac{2\sin(la)cos(la)}{2l} + a\right) \\
&= B^2\left(\frac{-\sin^3(la)}{l\cos(la)} - \frac{\sin(la)\cos(la)}{l} + a\right) \\
&= B^2\left(\frac{-\sin^3(la)}{l\cos(la)} - \frac{\sin(la)\cos^2(la)}{l\cos(la)} + a\right) \\
&= B^2\left[a - \frac{\sin(la)}{l\cos(la)}\left(\sin^2(la) + \cos^2(la)\right)\right] \\
&= B^2\left[a - \frac{\sin(la)}{l\cos(la)}\right] = B^2\left(a - \frac{1}{l\cot(la)}\right) = B^2\left(a + \frac{1}{k}\right) \\
&\Rightarrow B = \frac{1}{\sqrt{a+\frac{1}{k}}},\ D = \frac{e^{ka}\sin(la)}{\sqrt{a+\frac{1}{\kappa}}},\ A = -\frac{e^{\kappa a}\sin(la)}{\sqrt{a+\frac{1}{k}}}
\end{aligned}
$$

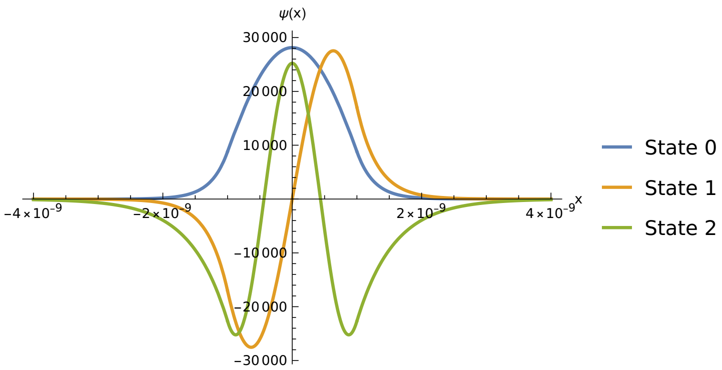
Plug in the parameters for each energy level, we have: For even bound state $n = 0, 2$:

$$
\psi_0(x) = \begin{cases} 3.93847\cdot 10^5 e^{(3.8\cdot 10^9 x)} & \text{if } x < -1\cdot 10^{-9}, \\ 28136.57\cos(1.2523\cdot 10^9 x) & \text{if } -1\cdot 10^{-9} \le x \le 1\cdot 10^{-9}, \\ 3.93847\cdot 10^5 e^{(-3.8\cdot 10^9 x)} & \text{if } x > 1\cdot 10^{-9}. \end{cases} \tag{10}
$$

$$
\psi_2(x) = \begin{cases} -1.3048\cdot 10^5 e^{(1.75\cdot 10^9 x)} & \text{if } x < -1\cdot 10^{-9}, \\ 25226\cos(3.5953\cdot 10^9 x) & \text{if } -1\cdot 10^{-9} \le x \le 1\cdot 10^{-9}, \\ -1.3048\cdot 10^5 e^{(-1.75\cdot 10^9 x)} & \text{if } x > 1\cdot 10^{-9}. \end{cases} \tag{11}
$$

For odd bound state $n = 1$:

$$
\psi_1(x) = \begin{cases} -393630 e^{(3.14\cdot 10^9 x)} & \text{if } x < -1\cdot 10^{-9}, \\ 27540.05\sin(2.47458\cdot 10^9 x) & \text{if } -1\cdot 10^{-9} \le x \le 1\cdot 10^{-9}, \\ 393630 e^{(-3.14\cdot 10^9 x)} & \text{if } x > 1\cdot 10^{-9}. \end{cases} \tag{12}
$$



(b) Wave Functions