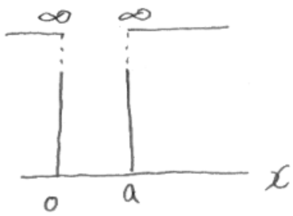
Quantum Mechanics (1 dimensional case)

1. Square Well Potential

1.1 Infinite Potential Case



① Set the equation :

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \rightarrow \quad \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

② Solve the differential equation :

$$\psi = A\sin\lambda x, \quad B\cos\lambda x \quad \left(\lambda = \frac{\sqrt{2mE}}{\hbar}\right)$$

③ Apply the boundary conditions to it :

When $x = 0$ and a, $\psi = 0$. Therefore $B = 0$,

and $A\sin\lambda x = 0$ $(A \neq 0)$. So $\lambda a = n\pi$. $(n = 1, 2, 3, \cdots)$

$$\therefore \quad \lambda = \frac{n\pi}{a}$$

The wave function is $\psi = A\sin\frac{n\pi}{a}x$

④ Normalize the wave function :

$$\int_0^a |\psi|^2 dx = 1$$

$$A^2\int_0^a \sin^2\frac{n\pi}{a}x\,dx = A^2\int_0^a\left(\frac{1}{2} - \frac{1}{2}\sin\frac{2n\pi}{a}x\right)dx$$

$$= A^2\left[\frac{x}{2} + \frac{a}{4n\pi}\cos\frac{2n\pi}{a}x\right]_0^a$$

$$= A^2\frac{a}{2}$$ But $\frac{A^2a}{2} = 1$, So $A = \sqrt{\frac{2}{a}}$.

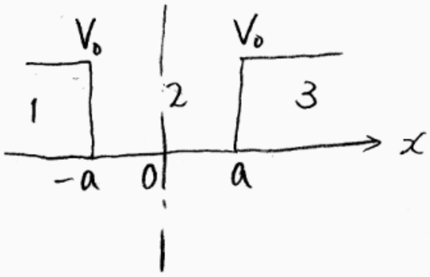
Therefore, $\psi = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x$

⑤ Find the energy eigen values :

$$\lambda = \frac{\sqrt{2mE}}{\hbar} \quad \text{and} \quad \lambda = \frac{n\pi}{a}$$

$$\therefore \quad E = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2}$$

1.2 Finite Potential Case I



① Set up the equations:

For 1 : $(\hbar^2/2m_0)\psi_1'' + (E-V_0)\psi_1 = 0$

For 2 : $(\hbar^2/2m_0)\psi_2'' + E\psi_2 = 0$

For 3 : $(\hbar^2/2m_0)\psi_3'' + (E-V_0)\psi_3 = 0$

② Solve the equations:

$$\left.\begin{aligned} \psi_1 &= Ce^{\beta x} + \cancel{C_1}^{\,0} e^{-\beta x} \\ \psi_2 &= A\sin\alpha x + B\cos\alpha x \\ \psi_3 &= De^{-\beta x} + \cancel{D_1}^{\,0} e^{\beta x} \end{aligned}\right\} \text{ where } \left\{\begin{aligned} \alpha &= \sqrt{2m_0E}/\hbar \\ \beta &= \sqrt{2m_0(V_0-E)}/\hbar \end{aligned}\right.$$

It is assumed that the system is a bound state. So when $x \to \pm\infty$, ψ_1 and $\psi_3 \longrightarrow 0$. In other words, α and β are not imaginary numbers. Therefore, $V_0 > E$ and $C_1 = 0$, $D_1 = 0$.

③ Boundary conditions:

when $x=-a$, $\psi_1 = \psi_2$: $-A\sin\alpha a + B\cos\alpha a = Ce^{-\beta a}$ ($\because$ $\sin(-a\alpha) = -\sin$ ... $\cos(-a\alpha) = \cos a\alpha$)

also $\psi_1' = \psi_2'$: $\alpha A\cos\alpha a + \alpha B\sin\alpha a = \beta Ce^{-\beta a}$

when $x = a$, $\psi_2 = \psi_3$: $A\sin\alpha a + B\cos\alpha a = De^{-\beta a}$

also $\psi_2' = \psi_3'$: $\alpha A\cos\alpha a - \alpha B\sin\alpha a = -\beta De^{-\beta a}$

From those, we can get

$$2A\sin\alpha a = (D-C)e^{-\beta a}, \quad 2\alpha A\cos\alpha a = -\beta(D-C)e^{-\beta a}$$

$$2B\cos\alpha a = (C+D)e^{-\beta a}, \quad 2\alpha B\sin\alpha a = \beta(C+D)e^{-\beta a}$$

Then, $A \neq 0$, $D-C \neq 0$ $\rightarrow$ $\alpha\cot\alpha a = -\beta$

$B \neq 0$, $C+D \neq 0$ $\rightarrow$ $\alpha\tan\alpha a = \beta$

From those, if $A \neq 0$ and $B \neq 0$ simultaneously, then $\tan^2 \alpha a = -1$. But α will become an imaginary number. So either one should be zero.

(i) $A = 0$, $B \neq 0$, then $C = D$ and we have

$$\xi \tan \xi = \eta \qquad (\text{where } \alpha a = \xi,\ \beta a = \eta)$$

(ii) $A \neq 0$, $B = 0$, then $C = -D$ and we have

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

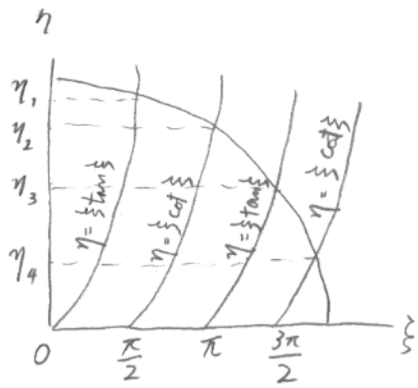
Recall $\alpha = \sqrt{2m_0 E}/\hbar$ and $\beta = \sqrt{2m_0(V_0 - E)}/\hbar$.

From those, we obtain

$$\alpha^2 + \beta^2 = \frac{2m_0 V_0}{\hbar^2}.$$

We can rewrite it as

$$\xi^2 + \eta^2 = \frac{2m_0 V_0 a^2}{\hbar^2}$$

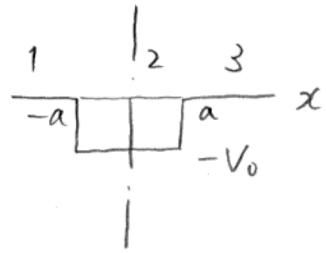


The intersections are the values of ξ and η.

And from $\alpha = \frac{\sqrt{2m_0 E}}{\hbar}$, $\quad E = \frac{\alpha^2 \hbar^2}{2m_0}$

namely, $$E = \frac{\hbar^2}{2m_0 a^2}\xi^2.$$

1.3 Finite Potential Case II



① Set up the equations :

For 1 , $(\hbar^2/2m_0)\,\psi_1'' + E\psi_1 = 0$

For 2, $(\hbar^2/2m_0)\,\psi_2'' + (E+V_0)\,\psi_2 = 0$

For 3, $(\hbar^2/2m_0)\,\psi_3'' + E\psi_3 = 0$

② Solve the equations :

$$\left.\begin{aligned} \psi_1 &= Ce^{\beta x} \\ \psi_2 &= A\sin\alpha x + B\cos\alpha x \\ \psi_3 &= De^{-\beta x} \end{aligned}\right\} \quad \text{where} \quad \alpha = \frac{\sqrt{2m_0(V_0+E)}}{\hbar}, \quad \beta = \frac{\sqrt{-2m_0E}}{\hbar}$$

For the bound state , β is not imaginary , so $E<0$.

Similarly to case I ,

$A \neq 0$, $D-C \neq 0 \longrightarrow \alpha\cot\alpha a = -\beta$

$B \neq 0$, $C+D \neq 0 \longrightarrow \alpha\tan\alpha a = \beta$

In other words,

$$\left.\begin{aligned} \xi\tan\xi &= \eta \\ \xi\cot\xi &= -\eta \end{aligned}\right\} \quad \text{where} \quad \left.\begin{aligned} \alpha a &= \xi \\ \beta a &= \eta \end{aligned}\right\}$$

Also

$$\alpha^2+\beta^2 = 2m_0V_0/\hbar \longrightarrow \xi^2+\eta^2 = \frac{2m_0V_0a^2}{\hbar^2}$$

However, from $\beta = \frac{\sqrt{-2m_0E}}{\hbar}$, we obtain

$$E = -\frac{\hbar^2}{2m_0a^2}\eta^2$$

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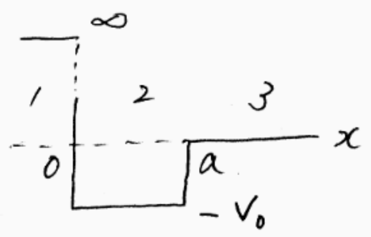
1.4 finite potential case III

① Set up the equations :



For 2, $(\hbar^2/2m_0)\psi_2'' + (E+V_0)\psi_2 = 0$

For 3, $(\hbar^2/2m_0)\psi_3'' + E\psi_3 = 0$

② Solve the equations :

$$\left.\begin{aligned} \psi_2 &= A\sin\alpha x + B\cos\alpha x \\ \psi_3 &= C e^{-\beta x} + C_1 e^{\beta x} \end{aligned}\right\} \quad \text{where} \quad \left\{\begin{aligned} \alpha &= \frac{\sqrt{2m_0(E+V_0)}}{\hbar} \\ \beta &= \frac{\sqrt{-2m_0E}}{\hbar} \end{aligned}\right.$$

From the bound state, $E<0$ and $C_1 = 0$.

Also, when $x=0$, ψ_2 must zero. Namely, $B=0$.

③ Boundary conditions

When $x=a$, $\psi_2 = \psi_3 \rightarrow A\sin\alpha a = Ce^{-\beta a}$

$\psi_2' = \psi_3' \rightarrow A\alpha\cos\alpha a = -C\beta e^{-\beta a}$

Therefore, $\alpha\cot\alpha a = -\beta$

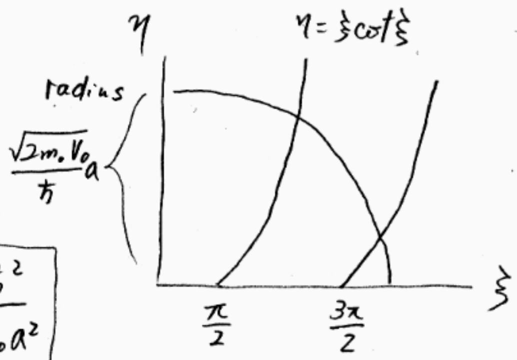
Put $\alpha a = \xi$ and $\beta a = \eta$.

$$\xi\cot\xi = -\eta \qquad \text{———} \quad (A)$$

④ Find the bound state.

$$\alpha^2 + \beta^2 = \frac{2m_0V_0}{\hbar^2} \rightarrow \xi^2 + \eta^2 = \frac{2m_0V_0}{\hbar^2}a^2 \quad \text{—} \ (B)$$

(A) and (B) on graph.



To get at least one bound state, the condition is :

$$\frac{\sqrt{2m_0V_0}}{\hbar}a \geq \frac{\pi}{2} \quad \therefore \quad \boxed{V_0 \geq \frac{\pi^2\hbar^2}{8m_0a^2}}$$