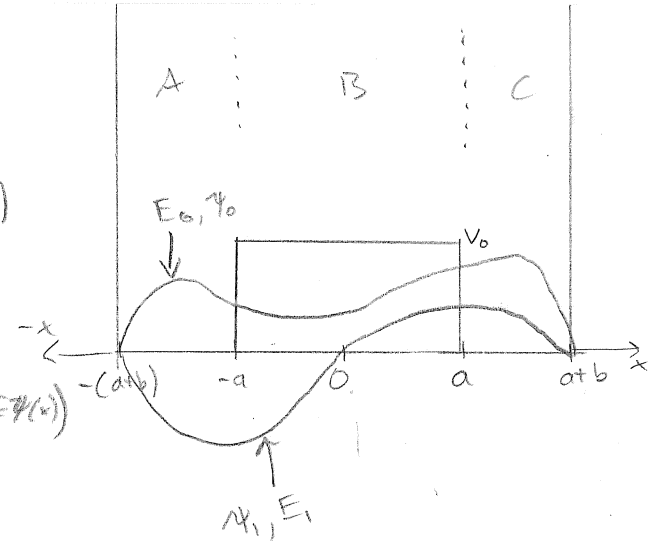


## 4.6 Boundary Conditions

$$\psi(-a+b) = \psi(a+b) = 0$$

$$\psi_A(a) = \psi_B(a) \quad \frac{d}{dx} \psi_A(-a) = \frac{d}{dx} \psi_B(-a)$$

$$\psi_B(a) = \psi_C(a) \quad \frac{d}{dx} \psi_B(a) = \frac{d}{dx} \psi_C(a)$$



### Schrödinger Equation

Regions

$$A: \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi_A(x) = E \psi_A(x)$$

$$B: \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi_B(x) + V_0 \psi_B(x) = E \psi_B(x)$$

$$C: \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \psi_C(x) = E \psi_C(x)$$

Solutions to the Schrödinger Eq in the Even case ( $\psi_0$ )

$$\psi_A(x) = e^{ikx}, \text{ but to match the boundary condition } \psi(-a+b) = 0,$$

$$\text{we choose } \psi_{0A}(x) = C_1 \sin(k(x+(a+b))) \quad \text{where } k = \sqrt{\frac{2m}{\hbar^2} E}$$

$$\text{also, } \psi_{0C}(x) = -C_1 \sin(k(x-(a+b))) = \psi_{0A}(-x) \quad \text{due to symmetry}$$

The solution for  $\psi_B(x)$  is a little trickier due to the damping.

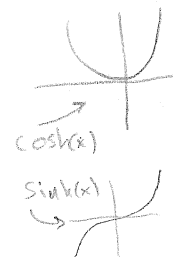
$$\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_B(x) = (V_0 - E) \psi_B(x) \Rightarrow \psi_B''(x) - \frac{2m}{\hbar^2} (V_0 - E) \psi_B(x) = 0$$

$$\text{The solutions are } \psi_B(x) = C_2 \sinh(k_0 x) + C_3 \cosh(k_0 x)$$

$$\text{where I let } k_0 \equiv \sqrt{\frac{2m}{\hbar^2} (V_0 - E)}$$

→ for even parity,  $\psi_B(x) = \psi_B(-x)$ ; so only  $\cosh$  survives.

$$\text{in all } \psi_0 = \begin{cases} C_1 \sin(k(x-(a+b))) & -(a+b) < x < -a & (A) \\ C_3 \cosh(k_0 x) & -a < x < a & (B) \\ -C_1 \sin(k(x+(a+b))) & a < x < a+b & (C) \end{cases}$$



### Solutions for the Odd case ( $\psi_1$ )

$$\text{Similarly, } \psi_1 = \begin{cases} -C_1 \sin(k(x-(a+b))) & -(a+b) < x < -a & (A) \\ C_3 \sinh(k_0 x) & -a < x < a & (B) \\ -C_1 \sin(k(x+(a+b))) & a < x < a+b & (C) \end{cases}$$

Now, we match boundary conditions

we'll use the RHS of the well b/c it's easier to think about.

$$\Psi_B(a) = \Psi_C(a) \Rightarrow \frac{\Psi_B(a)}{\Psi_C(a)} = 1 \quad \text{and} \quad \Psi_B'(a) = \Psi_C'(a) \Rightarrow \frac{\Psi_B'(a)}{\Psi_C'(a)} = 1$$

$$\Rightarrow \frac{\Psi_B'(0)}{\Psi_B(a)} = \frac{\Psi_C'(a)}{\Psi_C(a)}$$

{ 10/20 }

→ Even parity ( $\Psi_0$  case)

$$\frac{k_0 C_3 \sinh(k_0 a)}{C_3 \cosh(k_0 a)} = \frac{+k C_1 \cos(k(-a+a+b))}{-C_1 \sin(k(-a+a+b))} \Rightarrow k_0 \tanh(k_0 a) = -k \cot(kb)$$

Since  $V_0 \gg 1$ ,  $k_0 \gg 1$  as well.

Note  $\tanh(x) \approx (1 - e^{-2x})$  when  $x \gg 1$

Thus, we have

$$k_0(1 - 2e^{-2k_0 a}) = -k \cot(kb)$$

Let's consider the case where  $V_0 \rightarrow \infty$ . Then  $k_0 \rightarrow \infty$  too,

and  $k_0 = -k \cot(kb)$

In this limit,  $k_0 \rightarrow \infty$ , but  $-k \cot(kb)$  only goes to infinity at  $kb = \pi$

Thus  $k = \frac{\pi}{b}$

Back to the real world of  $V_0 \gg 1$ , but finite. We'll assume  $k \approx \frac{\pi - \delta}{b}$

$$k_0(1 - 2e^{-2k_0 a}) \approx -\frac{\pi}{b} \frac{\cos(\pi)}{\sin(\pi)} = +\frac{\pi}{b} \frac{1}{\sin(\pi)} \approx \frac{\pi}{b\delta}, \text{ where } \delta \ll 1.$$

$$\therefore k_0(1 - 2e^{-2k_0 a}) = \frac{\pi}{b\delta} \Rightarrow \delta = \frac{\pi}{k_0 b (1 - 2e^{-2k_0 a})}$$

$$\text{So } k \approx \frac{\pi - \frac{\pi}{k_0 b (1 - 2e^{-2k_0 a})}}{b} \approx \frac{\pi}{b} \left( 1 - \frac{1}{k_0 b} (1 + 2e^{-2k_0 a}) \right) \text{ since } k_0 \gg 1.$$

$$\text{Now, noting } k = \sqrt{\frac{2mE_0}{\hbar^2}} \Rightarrow E_0 = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2mb^2} \left( 1 + \frac{1}{k_0 b} (1 - 2e^{-2k_0 a}) \right)^2$$

finally,  $(1-x)^2 \approx 1 - 2x$ , when  $x \ll 1$ , and in this case  $\frac{1}{k_0 b} (1 + 2e^{-2k_0 a}) \ll 1$

$$\text{So } E_0 = \frac{\hbar^2 \pi^2}{2mb^2} \left( 1 - \frac{2}{k_0 b} (1 + 2e^{-2k_0 a}) \right)$$

20/20

→ Odd Parity ( $\Psi_1$  case) This is a lot of writing. In my search web,

I found VERY similarly that  $E_1 = \frac{\hbar^2 \pi^2}{2mb^2} \left( 1 - \frac{2}{k_0 b} (1 - 2e^{-2k_0 a}) \right)$

$$E_0 - E_1 = \frac{\hbar^2 \pi^2}{2mb^2} \left[ \frac{-2}{k_0 b} (1 + 2e^{-2k_0 a} - 1 + 2e^{-2k_0 a}) \right] = \frac{4\hbar^2 \pi^2}{mb^3 k_0} e^{-2k_0 a}$$

↑  
minus sign  
b/c  $\coth(k_0 a) \approx \frac{1 + 2e^{-2k_0 a}}{1 - 2e^{-2k_0 a}}$

95  
200