

Chapter 3

Particle in Box (PIB) Models

Homework Solutions

$$1. \quad y = Ae^{\alpha x} + Be^{-\alpha x} ; \quad \frac{dy}{dx} = \alpha Ae^{\alpha x} - \alpha Be^{-\alpha x} ; \quad \frac{d^2 y}{dx^2} = \alpha^2 Ae^{\alpha x} + \alpha^2 Be^{-\alpha x} = \alpha^2 y$$

$$\frac{d^2 y}{dx^2} - 4y = 0 \rightarrow \alpha^2 y - 4y = 0 \rightarrow \alpha = \sqrt{4} = 2$$

(No need to consider $\alpha = -2$, which would just reverse the A and B terms in the solution.)

Boundary Conditions

$$y(0) = 2 \rightarrow Ae^0 + Be^0 = 2 \rightarrow A + B = 2$$

$$y'(0) = 4 \rightarrow 2Ae^0 - 2Be^0 = 4 \rightarrow A - B = 2$$

$$\text{Add the two eqns to get: } 2A = 4 \rightarrow A = 2$$

$$B = 2 - A = 0 \rightarrow B = 0$$

$$\text{Solution: } y = 2e^{2x}$$

$$2. \quad a = 8 \text{ Ang} \cdot \frac{1 \times 10^{-10} \text{ m}}{1 \text{ Ang}} = 8 \times 10^{-10} \text{ m} \quad m_{H_2} = 2.00 \text{ amu} \cdot \frac{1.66 \times 10^{-27} \text{ kg}}{1 \text{ amu}} = 3.32 \times 10^{-27} \text{ g E}$$

$$E_1 = \frac{(1)^2 h^2}{8m_{H_2} a^2} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(3.32 \times 10^{-27} \text{ kg})(8 \times 10^{-10} \text{ m})^2} = 2.59 \times 10^{-23} \frac{\text{J}^2 \cdot \text{s}^2}{\text{kg} \cdot \text{m}^2}$$

$$(a) \quad = 2.59 \times 10^{-23} \frac{J \left(\frac{\text{kg} \cdot \text{m}^2}{\text{s}^2} \right) \cdot \text{s}^2}{\text{kg} \cdot \text{m}^2} = 2.59 \times 10^{-23} \text{ J}$$

$$(b) \quad E_1 = \frac{1}{2} m_{H_2} v^2 \rightarrow v = \sqrt{\frac{2 \cdot E_1}{m_{H_2}}} = \sqrt{\frac{2 \cdot 2.59 \times 10^{-23} \text{ kg} \cdot \text{m}^2 / \text{s}^2}{3.32 \times 10^{-27} \text{ kg}}} = 125 \text{ m/s}$$

$$(c) \quad E_n = \frac{1}{2} m_{H_2} v^2 = \frac{1}{2} (3.32 \times 10^{-27} \text{ kg}) (1.5 \times 10^5 \text{ m/s})^2 = 3.735 \times 10^{-17} \text{ kg} \cdot \text{m}^2 / \text{s}^2 = 3.735 \times 10^{-17} \text{ J}$$

$$E_n = \frac{n^2 h^2}{8m_{H_2} a^2}$$

$$n^2 = \frac{8m_{H_2} a^2 E_n}{h^2} = \frac{8(3.32 \times 10^{-27} \text{ kg})(8 \times 10^{-10} \text{ m})^2 (3.735 \times 10^{-17} \text{ J})}{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}$$

$$= 1.44 \times 10^8 \frac{\text{kg} \cdot \text{m}^2 \cdot \text{J}}{\left(\frac{\text{kg} \cdot \text{m}^2}{\text{s}^2} \right) \text{J} \cdot \text{s}^2} = 1.44 \times 10^6$$

$$n = \sqrt{1.44 \times 10^6} = 1.20 \times 10^3 = 1,200$$

3. $\lambda = 500 \text{ nm} = 5.0 \times 10^{-7} \text{ m}$

$$\Delta E = E_{\text{phot}} = h\nu = \frac{hc}{\lambda} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{5.00 \times 10^{-7} \text{ m}} = 3.98 \times 10^{-19} \text{ J}$$

$$\Delta E = \frac{n_U^2 h^2}{8ma^2} - \frac{n_L^2 h^2}{8ma^2} = (5^2 - 2^2) \frac{h^2}{8ma^2} = \frac{21h^2}{8ma^2}$$

$$a^2 = \frac{21h^2}{8m\Delta E} = \frac{21(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(9.11 \times 10^{-31} \text{ kg})(3.98 \times 10^{-19} \text{ J})} = 3.18 \times 10^{-18} \frac{\text{J} \cdot \text{s}^2}{\text{kg}}$$

$$= 3.18 \times 10^{-18} \frac{\left(\frac{\text{kg} \cdot \text{m}^2}{\text{s}^2}\right) \text{s}^2}{\text{kg}} = 3.18 \times 10^{-18} \text{ m}^2$$

$$a = \sqrt{3.18 \times 10^{-18} \text{ m}^2} = 1.78 \times 10^{-9} \text{ m} \approx 1.8 \text{ nm}$$

4. $\psi_1 = A \sin\left(\frac{1\pi x}{a}\right) = A \sin(\beta x) \quad , \quad \beta = \frac{\pi}{a}$

$$\psi_3 = A \sin\left(\frac{3\pi x}{a}\right) = A \sin(\alpha x) \quad , \quad \alpha = \frac{3\pi}{a} \quad \alpha - \beta = \frac{2\pi}{a} \quad , \quad \alpha + \beta = \frac{4\pi}{a}$$

$$\int_0^a \psi_1^* \psi_3 dx = A^2 \int_0^a \sin(\alpha x) \sin(\beta x) dx = A^2 \left\{ \frac{\sin[(\alpha - \beta)x]}{2(\alpha - \beta)} - \frac{\sin[(\alpha + \beta)x]}{2(\alpha + \beta)} \right\}_0^a$$

$$= A^2 \left\{ \frac{\sin[(2\pi/a)x]}{2(\alpha - \beta)} - \frac{\sin[(4\pi/a)x]}{2(\alpha + \beta)} \right\}_0^a = A^2 \left[\frac{\sin(2\pi)}{2(\alpha - \beta)} - \frac{\sin(4\pi)}{2(\alpha + \beta)} \right] - A^2 \left[\frac{\sin(0)}{2(\alpha - \beta)} - \frac{\sin(0)}{2(\alpha + \beta)} \right] = 0 - 0 = 0$$

5. (a) Normalization

$$1 = \int_0^a \psi^2 dx = \int_0^a \{Ax^2(a-x)\}^2 dx = A^2 \int_0^a \{x^4(a-x)^2\} dx = A^2 \int_0^a \{a^2 x^4 - 2ax^5 + x^6\} dx$$

$$1 = A^2 \left\{ a^2 \left[\frac{x^5}{5} \right]_0^a - 2a \left[\frac{x^6}{6} \right]_0^a + \left[\frac{x^7}{7} \right]_0^a \right\} = A^2 \left\{ \frac{a^7}{5} - \frac{a^7}{3} + \frac{a^7}{7} \right\}$$

$$= A^2 \left\{ \frac{21a^7 - 35a^7 + 15a^7}{5 \cdot 3 \cdot 7} \right\} = A^2 \frac{a^7}{105} \rightarrow A = \sqrt{\frac{105}{a^7}}$$

(b) $P(0 \leq x \leq 0.40a)$

$$\begin{aligned}
 P(0 \leq x \leq 0.40a) &= \int_0^{0.40a} \psi^2 dx = \int_0^{0.40a} \{Ax^2(a-x)\}^2 dx = A^2 \int_0^{0.40a} \{x^4(a-x)^2\} dx \\
 &= A^2 \int_0^{0.40a} \{a^2x^4 - 2ax^5 + x^6\} dx = A^2 \left\{ a^2 \left[\frac{x^5}{5} \right]_0^{0.40a} - 2a \left[\frac{x^6}{6} \right]_0^{0.40a} + \left[\frac{x^7}{7} \right]_0^{0.40a} \right\} \\
 &= A^2 \left\{ a^2 \left[\frac{(0.40a)^5}{5} \right] - 2a \left[\frac{(0.40a)^6}{6} \right] + \left[\frac{(0.40a)^7}{7} \right] \right\} \\
 &= A^2 \left\{ (2.048 \times 10^{-3})a^7 - (1.365 \times 10^{-3})a^7 + (2.341 \times 10^{-4})a^7 \right\} \\
 &= \left(\frac{105}{a^7} \right) (9.171 \times 10^{-4} a^7) = 0.0962 \approx 0.096
 \end{aligned}$$

(c) $\langle x^2 \rangle$

$$\begin{aligned}
 \langle x^2 \rangle &= \int_0^a x^2 \psi^2 dx = \int_0^a x^2 \{Ax^2(a-x)\}^2 dx = A^2 \int_0^a x^4 \{a^2x^2 - 2ax^3 + x^4\} dx \\
 &= A^2 \int_0^a \{a^2x^6 - 2ax^7 + x^8\} dx = A^2 \left\{ a^2 \left[\frac{x^7}{7} \right]_0^a - 2a \left[\frac{x^8}{8} \right]_0^a + \left[\frac{x^9}{9} \right]_0^a \right\} \\
 &= \left(\frac{105}{a^7} \right) \left\{ \frac{a^9}{7} - \frac{a^9}{4} + \frac{a^9}{9} \right\} = \left(\frac{105}{a^7} \right) \left\{ \frac{36a^9 - 63a^9 + 28a^9}{7 \cdot 4 \cdot 9} \right\} \\
 &= \left(\frac{105}{a^7} \right) \left\{ \frac{1a^9}{252} \right\} = \frac{105}{252} a^2 = 0.417 a^2
 \end{aligned}$$

(d) $\langle E \rangle$: Since $E = p^2/2m$, $\hat{E} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$

$$\text{Preliminary: } \frac{d^2\psi}{dx^2} = \frac{d}{dx} \left[\frac{d}{dx} \{Aax^2 - Ax^3\} \right] = \frac{d}{dx} [2aAx - 3Ax^2] = 2aA - 6Ax = A(2a - 6x)$$

$$\begin{aligned}
 \langle E \rangle &= \int_0^a \psi^* \hat{E} \psi dx = \int_0^a \psi^* \left(-\frac{\hbar^2}{2m} \right) \frac{d^2\psi}{dx^2} dx = \int_0^a [Ax^2(a-x)] \left(-\frac{\hbar^2}{2m} \right) [A(2a-6x)] dx \\
 &= \left(-\frac{\hbar^2 A^2}{2m} \right) \int_0^a [x^2(a-x)(2a-6x)] dx = \left(-\frac{\hbar^2 A^2}{2m} \right) \int_0^a [2a^2x^2 - 8ax^3 + 6x^4] dx \\
 &= \left(-\frac{\hbar^2 A^2}{2m} \right) \left\{ 2a^2 \left[\frac{x^3}{3} \right]_0^a - 8a \left[\frac{x^4}{4} \right]_0^a + 6 \left[\frac{x^5}{5} \right]_0^a \right\} = \left(-\frac{\hbar^2 A^2}{2m} \right) \left\{ 2 \frac{a^5}{3} - 2a^5 + 6 \frac{a^5}{5} \right\} \\
 &= \left(-\frac{\hbar^2 A^2}{2m} \right) \left[\frac{10a^5 - 30a^5 + 18a^5}{15} \right] = -\left(\frac{105}{a^7} \right) \left(\frac{\hbar^2}{4\pi^2} \right) \left(\frac{1}{2m} \right) \left(-\frac{2a^5}{15} \right) \\
 \langle E \rangle &= \frac{7}{4\pi^2} \frac{\hbar^2}{ma^2} = 0.177 \frac{\hbar^2}{ma^2}
 \end{aligned}$$

6. 1,3,5-hexatriene: There are 5 CC bonds.

The average bond length is estimated as $R = 0.14 \text{ nm}$

The box length is: $a = 5R + 2(1/2)R = 6R = 6(0.14 \text{ nm}) = 0.84 \text{ nm} = 8.4 \times 10^{-10} \text{ m}$.

In the ground state, $n = 1, 2$, and 3 levels are occupied.

The lowest transition is from $n = 3$ to $n = 4$.

$$\Delta E = \frac{n_u^2 h^2}{8ma^2} - \frac{n_l^2 h^2}{8ma^2} = (4^2 - 3^2) \frac{h^2}{8ma^2} = 7 \frac{h^2}{8ma^2} =$$

$$7 \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(9.11 \times 10^{-31} \text{ kg})(8.40 \times 10^{-10} \text{ m})^2} = 5.98 \times 10^{-19} \text{ J}$$

$$E_{\text{phot}} = \frac{hc}{\lambda} \rightarrow \lambda = \frac{hc}{E_{\text{phot}}} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{5.98 \times 10^{-19} \text{ J}} = 3.32 \times 10^{-7} \text{ m} = 332 \text{ nm}$$

7. $a = b = 0.35 \text{ nm} = 3.5 \times 10^{-10} \text{ m}$ $m = m_e = 9.11 \times 10^{-31} \text{ kg}$

See PP Section on Two-Dimensional PIB

$$\text{Energy Levels for Square Box: } E_{n_x, n_y} = \frac{h^2}{8ma^2} (n_x^2 + n_y^2)$$

The lowest four energy levels correspond to:

$n_x = n_y = 1$, $n_x = 2, n_y = 1$, $n_x = 1, n_y = 2$, $n_x = 2, n_y = 2$ (See diagram in PP)

The six electrons occupy the lowest 3 energy levels. The lowest $\pi \rightarrow \pi^*$ transition corresponds to $n_x = 2, n_y = 1 \rightarrow n_x = 2, n_y = 2$

$$\Delta E = E_{2,2} - E_{2,1} = \frac{h^2}{8ma^2} (2^2 + 2^2) - \frac{h^2}{8ma^2} (2^2 + 1^2) = 3 \frac{h^2}{8ma^2}$$

$$E_{\text{phot}} = \Delta E = 3 \frac{h^2}{8ma^2} = 3 \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(9.11 \times 10^{-31} \text{ kg})(3.5 \times 10^{-10} \text{ m})^2} = 1.48 \times 10^{-18} \text{ J}$$

$$E_{\text{phot}} = \frac{hc}{\lambda} \rightarrow \lambda = \frac{hc}{E_{\text{phot}}} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{1.48 \times 10^{-18} \text{ J}} = 1.34 \times 10^{-7} \text{ m} = 134 \text{ nm}$$

$$\lambda(\text{exp}) = 180 \text{ nm}$$

8.
$$E_{n_x, n_y} = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8mb^2} = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8m(2a)^2} = \frac{4n_x^2 h^2}{32ma^2} + \frac{n_y^2 h^2}{32ma^2} = \frac{(4n_x^2 + n_y^2)}{32} \cdot \frac{h^2}{ma^2}$$

Level #	n_x	n_y	E / (h^2/ma^2)
1	1	1	5/32 = 0.156
2	1	2	8/32 = 0.250
3	1	3	13/32 = 0.406
4	2	1	17/32 = 0.531
5	1	4	20/32 = 0.625
5	2	2	20/32 = 0.625
6	2	3	25/32 = 0.781
7	1	5	29/32 = 0.906
8	3	1	37/32 = 1.16

9.
$$M(\text{NO}_2) = 46 \text{ amu} \rightarrow m = 46 \text{ amu} \cdot \frac{1.66 \times 10^{-27} \text{ kg}}{1 \text{ amu}} = 7.64 \times 10^{-26} \text{ kg}$$

$$T = 100^\circ\text{C} = 373 \text{ K}, n = 3 \text{ mol}, p = 0.50 \text{ atm} \cdot \frac{1.013 \times 10^5 \text{ Pa}}{1 \text{ atm}} = 5.065 \times 10^4 \text{ Pa}$$

Preliminary Calculations: Partition Function

$$V = \frac{nRT}{P} = \frac{(3 \text{ mol})(8.31 \text{ kPa} \cdot \text{m}^3 / \text{mol} \cdot \text{K})(373 \text{ K})}{5.065 \times 10^4 \text{ Pa}} = 0.184 \text{ m}^3$$

$$q^{\text{tran}} = \left[\frac{2\pi mkT}{h^2} \right]^{3/2} V = \left[\frac{2(3.14)(7.64 \times 10^{-26} \text{ kg})(1.38 \times 10^{-23} \text{ J / K})(373 \text{ K})}{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2} \right]^{3/2} (0.184 \text{ m}^3)$$

$$= 7.75 \times 10^{31}$$

$$Q^{\text{tran}} = \frac{(q^{\text{tran}})^N}{N!} = (q^{\text{tran}})^N \frac{e^N}{N^N} = \left[\frac{q^{\text{tran}} \cdot e}{N} \right]^N$$

$$\ln(Q^{\text{tran}}) = \ln \left[\frac{q^{\text{tran}} \cdot e}{N} \right]^N = N \ln \left[\frac{q^{\text{tran}} \cdot e}{N} \right] = nN_A \ln \left[\frac{q^{\text{tran}} \cdot e}{nN_A} \right]$$

$$= 3 \text{ mol} (6.02 \times 10^{23} \text{ mol}^{-1}) \ln \left[\frac{(7.75 \times 10^{31})(2.72)}{(3 \text{ mol})(6.02 \times 10^{23} \text{ mol}^{-1})} \right]$$

$$= 3.35 \times 10^{25}$$

Preliminary Calculations: Partition Function Derivatives

$$\ln(Q^{tran}) = \ln \left[\frac{\left(\frac{2\pi mkT}{h^2} \right)^{3/2} \cdot V \cdot e}{N} \right]^N$$
$$= 3N / 2 \cdot \ln(2\pi mk / h^2) + 3N / 2 \cdot \ln(T) + N \ln(V) + N - N \ln(N)$$

$$\left(\frac{\partial \ln(Q^{tran})}{\partial T} \right)_{V,N} = \frac{3N}{2T} = \frac{3nN_A}{2T}$$

$$\left(\frac{\partial \ln(Q^{tran})}{\partial \ln(V)} \right)_{T,N} = N = nN_A$$

Internal Energy: U^{tran}

$$U^{tran} = kT^2 \left(\frac{\partial \ln Q^{tran}}{\partial T} \right)_{V,N} = kT^2 \left[\frac{3nN_A}{2T} \right] = \frac{3}{2}(n)(kN_A)T = \frac{3}{2}nRT$$
$$= \frac{3}{2}(3mol)(8.31 J / mol \cdot K)(373 K) = 13,950 J \approx 14.0 kJ$$

Constant volume Heat Capacity: $(C_V)^{tran}$

$$C_V^{tran} = \left(\frac{\partial U^{tran}}{\partial T} \right)_{V,N} = \left(\frac{\partial \left[\frac{3}{2} nRT \right]}{\partial T} \right)_{V,N} = \frac{3}{2} nR = \frac{3}{2}(3mol)(8.31 J / mol \cdot K)$$
$$= 37.4 J / mol \cdot K$$

Enthalpy: H^{tran}

$$H^{tran} = kT^2 \left(\frac{\partial \ln Q^{tran}}{\partial T} \right)_{V,N} + kT \left(\frac{\partial \ln Q^{tran}}{\partial \ln V} \right)_{T,N} = U^{tran} + kT \left(\frac{\partial \ln Q^{tran}}{\partial \ln V} \right)_{T,N}$$
$$= \frac{3}{2}nRT + kT(nN_A) = \frac{3}{2}nRT + nRT = \frac{5}{2}nRT = \frac{5}{2}(3mol)(8.31 J / mol \cdot K)(373 K)$$
$$= 23250 J \approx 23.3 kJ$$

Entropy: S^{tran}

$$S^{tran} = k \ln Q^{tran} + \frac{U^{tran}}{T} = (1.38 \times 10^{-23} J / K)(3.35 \times 10^{25}) + \frac{13950 J}{373 K}$$
$$= 462.3 J / K + 37.4 J / K = 499.7 J / K \approx 500 J / K$$

Helmholtz Energy: A^{tran}

$$A^{\text{tran}} = -kT \ln(Q^{\text{tran}}) = (-1.38 \times 10^{-23} \text{ J / K})(373 \text{ K})(3.35 \times 10^{23})$$

$$= -172,400 \text{ J} \approx -172 \text{ kJ}$$

Gibbs Energy: G^{tran}

$$G^{\text{tran}} = -kT \ln Q^{\text{tran}} + kT \left(\frac{\partial \ln Q^{\text{tran}}}{\partial \ln V} \right)_{T,N} = A + kT (nN_A)$$

$$= A + nRT = -172,400 \text{ J} + (3 \text{ mol})(8.31 \text{ J / mol} \cdot \text{K})(373 \text{ K})$$

$$= -163,100 \text{ J} \approx -163 \text{ kJ}$$

10. $q^{\text{tran}}(\text{O}_2, 298 \text{ K}, 1 \text{ atm}) = 4.28 \times 10^{30}$

$$M(\text{O}_2) = 32 \text{ g/mol}$$

$$M(\text{Cl}_2) = 71 \text{ g/mol}$$

Let's determine how q^{trans} depends on M, T and P

$$q^{\text{tran}} = \left(\frac{2\pi mkT}{h^2} \right)^{3/2} V = \left(\frac{2\pi MkT}{N_A h^2} \right)^{3/2} \frac{nRT}{P} = C \frac{M^{3/2} T^{5/2}}{P}$$

(a) Cl_2 at 298 K and 1 atm

$$\frac{q^{\text{tran}}(\text{Cl}_2, 298 \text{ K}, 1 \text{ atm})}{q^{\text{tran}}(\text{O}_2, 298 \text{ K}, 1 \text{ atm})} = \left(\frac{M(\text{Cl}_2)}{M(\text{O}_2)} \right)^{3/2} = \left(\frac{71}{32} \right)^{3/2} = 3.30$$

$$q^{\text{tran}}(\text{Cl}_2, 298 \text{ K}, 1 \text{ atm}) = 3.30 \cdot q^{\text{tran}}(\text{O}_2, 298 \text{ K}, 1 \text{ atm})$$

$$= 3.30 (4.28 \times 10^{30}) = 1.41 \times 10^{31}$$

(b) O_2 at 1273 K and 1 atm

$$\frac{q^{\text{tran}}(\text{O}_2, 1273 \text{ K}, 1 \text{ atm})}{q^{\text{tran}}(\text{O}_2, 298 \text{ K}, 1 \text{ atm})} = \left(\frac{1273}{298} \right)^{5/2} = 37.7$$

$$q^{\text{tran}}(\text{O}_2, 1273 \text{ K}, 1 \text{ atm}) = 37.7 \cdot q^{\text{tran}}(\text{O}_2, 298 \text{ K}, 1 \text{ atm})$$

$$= 37.7 (4.28 \times 10^{30}) = 1.61 \times 10^{32}$$

(c) O₂ at 1273 K and 10 atm

$$\frac{q^{tran}(O_2, 1273 K, 10 atm)}{q^{tran}(O_2, 1273 K, 1 atm)} = \left(\frac{1/P_2}{1/P_1} \right) = \frac{P_1}{P_2} = \frac{1 atm}{10 atm} = 0.10$$

$$\begin{aligned} q^{tran}(O_2, 1273 K, 10 atm) &= 37.7 \cdot q^{tran}(O_2, 1273 K, 1 atm) \\ &= 0.10(1.61 \times 10^{32}) = 1.61 \times 10^{31} \end{aligned}$$

NOTE: Because we were calculating only ratios of M and P, it was not necessary to convert to SI Units

11.

$$\psi_1 = Ae^{+\alpha x} + Be^{-\alpha x}$$

$$\psi_2 = C \sin[\beta(L - x)] + D \cos[\beta(L - x)]$$

(a) Region 1: $\psi_1 = 0$ at $x = -\infty$

Boundary Condition

$$\psi_1(x = -\infty) = 0 = Ae^{+\alpha x} + Be^{-\alpha x} = Ae^{-\infty} + Be^{+\infty} = 0 + Be^{+\infty} \rightarrow B = 0$$

Therefore: $\psi_1 = Ae^{+\alpha x}$

$$\text{Schrödinger Equation: } -\frac{\hbar^2}{2m} \frac{d^2\psi_1}{dx^2} + V_1\psi_1 = E\psi_1 \rightarrow \frac{d^2\psi_1}{dx^2} = \frac{2m}{\hbar^2}(V_1 - E)\psi_1$$

$$\psi_1 = Ae^{+\alpha x}$$

$$\frac{d\psi_1}{dx} = A\alpha e^{+\alpha x}$$

$$\frac{d^2\psi_1}{dx^2} = \alpha^2 Ae^{+\alpha x} = \alpha^2 \psi_1$$

$$\frac{d^2\psi_1}{dx^2} = \frac{2m}{\hbar^2}(V_1 - E)\psi_1 \rightarrow \alpha^2 \psi_1 = \frac{2m}{\hbar^2}(V_1 - E)\psi_1 \rightarrow \alpha^2 = \frac{2m}{\hbar^2}(V_1 - E)$$

$$\text{Therefore: } \alpha = \sqrt{\frac{2m}{\hbar^2}(V_1 - E)}$$

(b) Region 2: $\psi_2 = 0$ at $x = L$

Boundary Condition

$$\psi_2(x = L) = 0 = C \sin[\beta(L - L)] + D \cos[\beta(L - L)] = C \sin(0) + D \cos(0) = D$$

$$\text{Therefore: } D = 0 \text{ and } \psi_2 = C \sin[\beta(L - x)] + D \cos[\beta(L - x)] = C \sin[\beta(L - x)]$$

$$\text{Schrödinger Equation: } -\frac{\hbar^2}{2m} \frac{d^2\psi_2}{dx^2} + V_2\psi_2 = E\psi_2 \rightarrow \frac{d^2\psi_2}{dx^2} = \frac{2m}{\hbar^2}(V_2 - E)\psi_2$$

$$\psi_2 = C \sin[\beta(L - x)]$$

$$\frac{d\psi_2}{dx} = -\beta C \cos[\beta(L - x)]$$

$$\frac{d^2\psi_2}{dx^2} = -\beta^2 C \sin[\beta(L - x)] = -\beta^2 \psi_2$$

$$\frac{d^2\psi_2}{dx^2} = \frac{2m}{\hbar^2}(V_2 - E)\psi_2 \rightarrow -\beta^2 \psi_2 = \frac{2m}{\hbar^2}(V_2 - E)\psi_2 \rightarrow \beta^2 = \frac{2m}{\hbar^2}(E - V_2)$$

$$\text{Therefore: } \beta = \sqrt{\frac{2m}{\hbar^2}(E - V_2)}$$

(c) Boundary Conditions at $x = 0$

$$\psi_1 = Ae^{+\alpha x} \quad \text{and} \quad \frac{d\psi_1}{dx} = \alpha Ae^{+\alpha x}$$

$$\psi_2 = C \sin[\beta(L - x)] \quad \text{and} \quad \frac{d\psi_2}{dx} = -\beta C \cos[\beta(L - x)]$$

$$\text{BC 1: } \psi_1(x = 0) = \psi_2(x = 0) \rightarrow C \sin[\beta(L - 0)] = Ae^{+\alpha 0}$$

$$\text{Therefore: } C \sin[\beta L] = A$$

$$\text{BC 2: } \left(\frac{d\psi_2}{dx} \right)_{x=0} = \left(\frac{d\psi_1}{dx} \right)_{x=0} \rightarrow -\beta C \cos[\beta(L - 0)] = \alpha Ae^0$$

$$\text{Therefore: } -\beta C \cos[\beta L] = \alpha A$$