One Dimensional Examples 1

Kaito Takahashi

Time Independent Hamiltonian

$$\hat{H}\psi(q_1, q_2, \ldots q_n, t) = i\eta \frac{\partial \psi(q_1, q_2, \ldots q_n, t)}{\partial t}$$

$$\psi(q_1, q_2, \ldots q_n, t) = \psi(q_1, q_2, \ldots q_n) Exp(-iEt/\eta)$$

$$\hat{H}\psi(q_1, q_2, \ldots q_n) = E\psi(q_1, q_2, \ldots q_n)$$

If the Hamiltonian Operator does not have time dependence then the time dependent problem is transferred to a time independent problem of finding the eigenfunction and eigenvalue of the Hamiltonian operator

Making Hamiltonian of Free Motion

Free Particle Motion: Particle moving with out any restriction by a potential

Has only kinetic energy called translational motion

Classical Hamiltonian

$$H = T = \frac{p_x^2}{2m}$$

$$\hat{P}_x = \frac{\eta}{i}\frac{d}{dx}\times$$

Quantum Hamiltonian Operator

$$\hat{H} = \frac{\hat{p}_x^2}{2m} = -\frac{\eta^2}{2m}\frac{d^2}{dx^2}$$

$$\hat{H}\psi(x) = -\frac{\eta^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

Solving Free Particle SE

$$\hat{H}\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

$$\psi_k(x) = AExp(ikx) + BExp(-ikx) \qquad\qquad E_k = \frac{k^2\hbar^2}{2m}$$

A,B are constants and k is the label for the eigenfunction and eigenvalue

k can take any value eigenvalues of free particle are continuous

Write the wavefunction as a function of cos and sin
What is the wave length of the wavefunction

Energy and Momentum

$$\left[\hat{H}, \hat{p}_x\right] = ???$$

$$\psi_k(x) = AExp(ikx) + BExp(-ikx)$$

If B=0

$$\hat{p}_x \psi_k(x) = \hat{p}_x AExp(ikx)$$
$$= \eta k AExp(ikx)$$
$$= \eta k \psi_k(x)$$

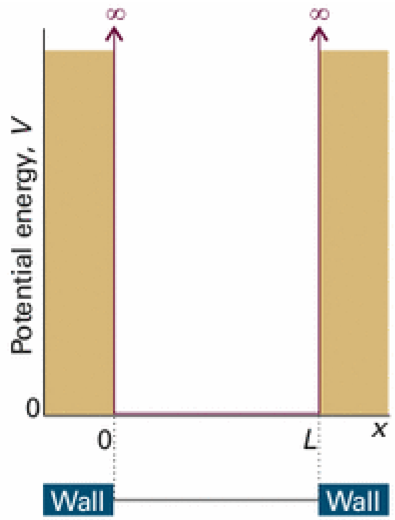
If A=0

$$\hat{p}_x \psi_k(x) = \hat{p}_x BExp(-ikx)$$
$$= -\eta k BExp(-ikx)$$
$$= -\eta k \psi_k(x)$$

$$E_k = \frac{k^2 \eta^2}{2m} \qquad k = \sqrt{\frac{2mE_k}{\eta^2}}$$

Wave function of the free translation motion has exact magnitude for momentum, but the direction is arbitrary depends on the value of the coefficients

Particle In a Box Hamiltonian



Motion of the particle limited by a wall

$$H = T + V = \frac{p_x^2}{2m} + V(x) \qquad \begin{array}{ll} V(x) = 0 & for\ \ 0 < x < L \\ V(x) = \infty & for\ \ x \leq 0, x \geq L \end{array}$$

Inside the box is free particle

$$\psi_k(x) = C\sin kx + D\cos kx \qquad\qquad E_k = \frac{k^2\eta^2}{2m}$$

If the potential energy is infinity there is 0 probability of existance

$$\psi_k(x) = 0 \qquad \text{for } x \leq 0 \text{ and} \geq \text{L}$$

Solving Particle in a Box

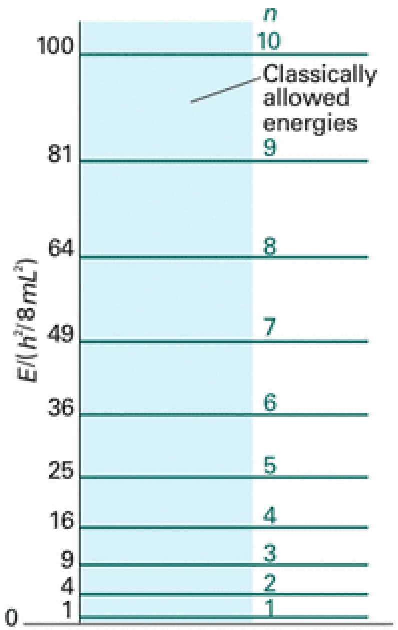
$$\psi_k(0) = C\sin 0 + D\cos 0 = D = 0$$

$$\psi_k(L) = C\sin kL = 0$$

$$k = \frac{n\pi}{L} \qquad n = 1,2,3,4....$$

Only integer values

n=0 is not allowed! Zero Point Energy



Eigenvalue defined by integer values of n

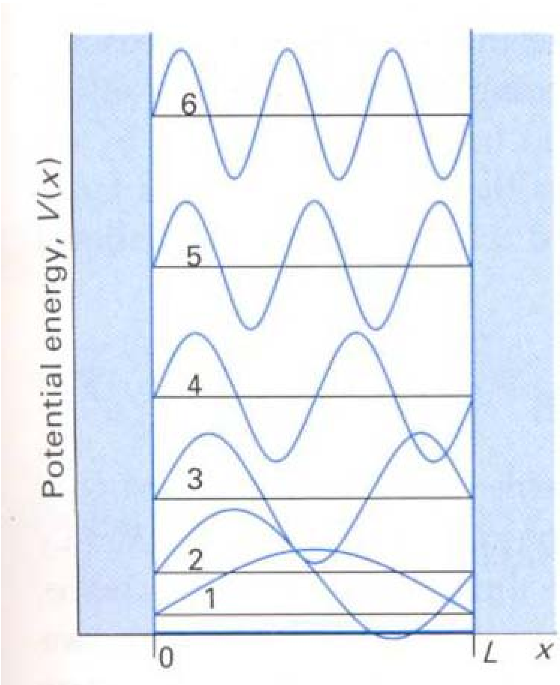
$$\psi_n(x) = C\sin\frac{n\pi}{L}x$$

$$E_n = \frac{n^2h^2}{8mL^2}$$

Obtain the normalization Constant C

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1 \qquad C = \sqrt{\frac{2}{L}}$$

Property of Solution



What is the average value of the position and momentum for the nth state?

$$\langle \hat{A} \rangle = \int \psi_n{}^*(x) \hat{A} \psi_n(x) dx$$

$$\langle \hat{x} \rangle = \frac{L}{2}$$

$$\langle \hat{p}_x \rangle = 0$$

What is the physical meaning of the above finding?

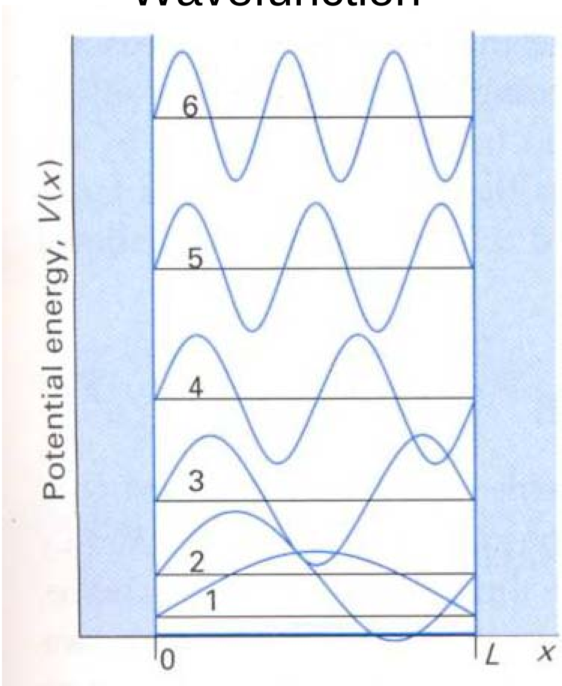
Orthogonality

Show that n=3 and n=4 wavefunctions are orthogonal

$$\int \psi_{n=3}^{*}(x)\psi_{n=4}(x)dx = 0$$

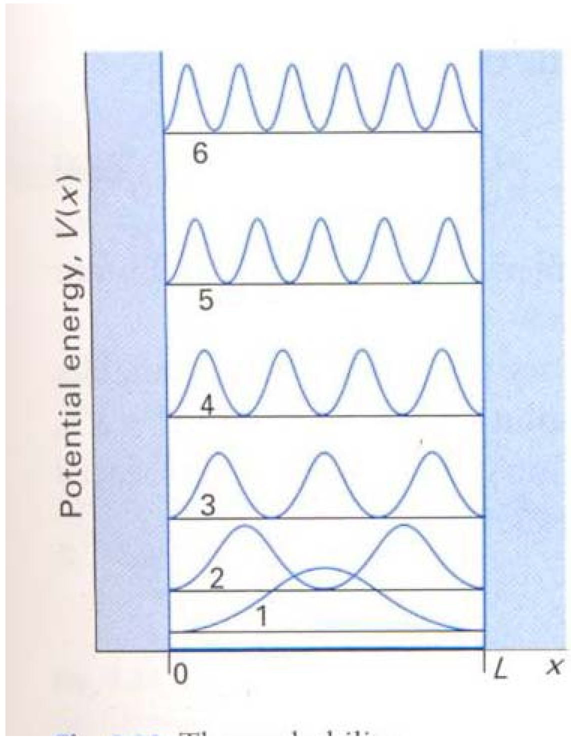
Correspondence to classical mechanics

Wavefunction



Notice that at low energies the distribution is localized however as the energy increases the distribution becomes closer to uniform distribution.
Which is closer to the classical picture?

Probability Density



Boundary Condition and Quantization

The energy is quantized due to the fact that the wavefunction is zero at boundaries

Box with a Constant Potential Energy

$$H = T + V = \frac{p_x^2}{2m} + V(x) \qquad V(x) = V \quad for\ \ 0 < x < L$$

$$V(x) = \infty \quad for\ \ x \le 0, x \ge L$$

$$for\ \ 0 < x < L \qquad \hat{H}\psi(x) = -\frac{\eta^2}{2m}\frac{d^2}{dx^2}\psi(x) + V\psi(x) = E\psi(x)$$

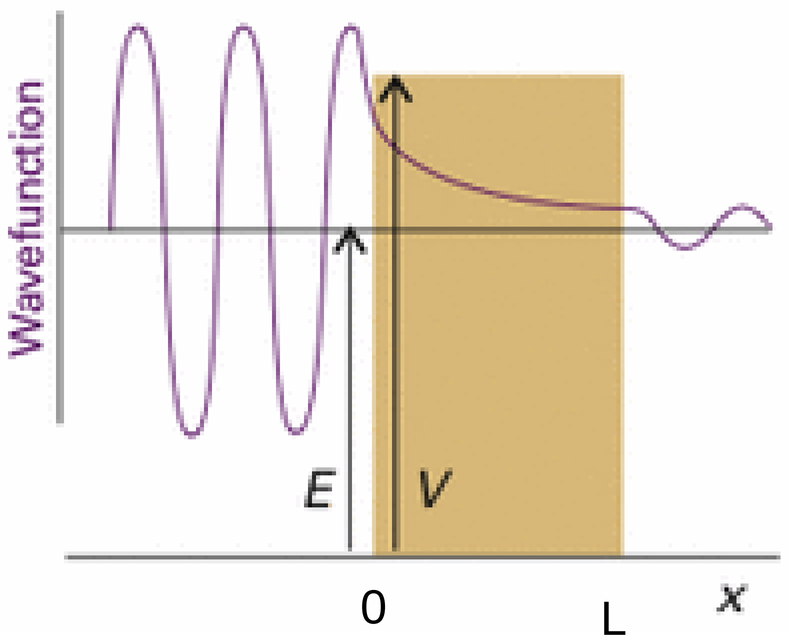
What is the solution for $E > V$?

If the potential energy is infinity there is 0 probability of existance

$$\psi_k(x) = 0 \qquad \text{for } x \le 0 \text{ and} \ge \text{L}$$

Penetration of a Barrier 1

$$zone\,1 \quad (x \le 0) \quad V(x) = 0$$
$$zone\,2 \quad (0 < x < L) \quad V(x) = V$$
$$zone\,3 \quad (x \ge L) \quad V(x) = 0$$



What are the general answer in each zone?

Zone 1

$$\psi_1(x) = AExp(ikx) + BExp(-ikx)$$
$$k\eta = \sqrt{2mE}$$

Zone 2

$$\psi_2(x) = A'Exp(ik'x) + B'Exp(-ik'x)$$
$$k'\eta = \sqrt{2m(E-V)}$$

Zone 3

$$\psi_3(x) = A''Exp(ikx) + B''Exp(-ikx)$$
$$k\eta = \sqrt{2mE}$$

Penetration of a Barrier 2

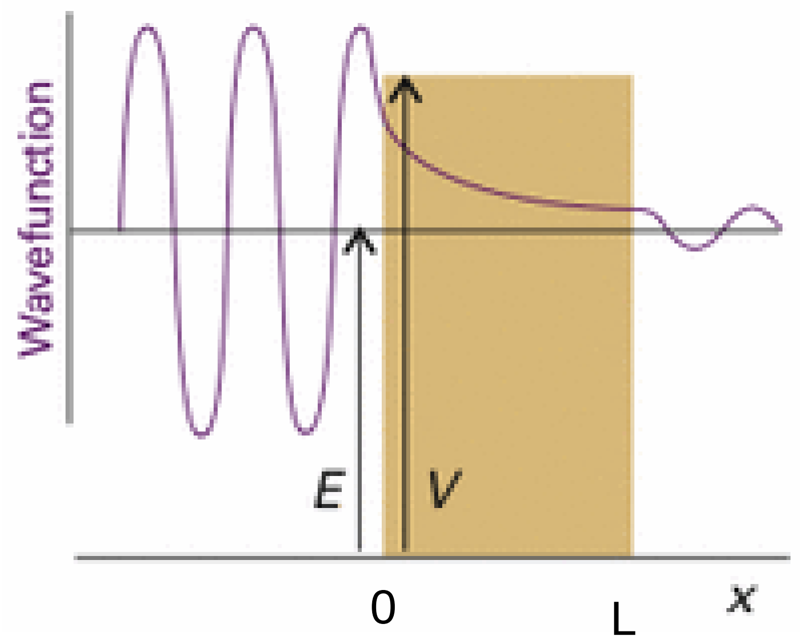
Consider E<V: In classical sense no transmission between zone 1 and zone3

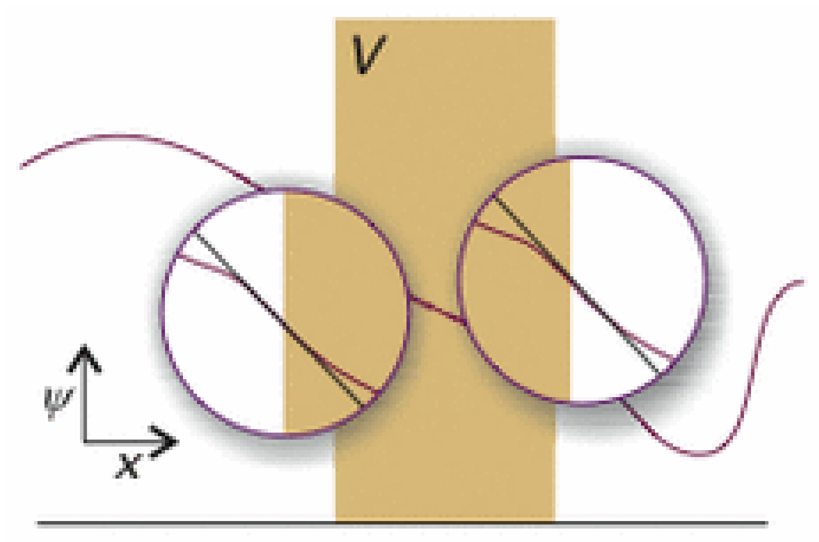
Zone 2

$$\psi_2(x) = A' Exp(-\kappa x) + B' Exp(\kappa x)$$

$$\kappa \eta = \sqrt{2m(V-E)}$$

How do we find values of coef? From the connection of wave function





Penetration of Barrier 3

Continuation of Wavefunction and its derivative

$$\psi_1(0) = \psi_2(0) \qquad \frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}$$

$$\psi_2(L) = \psi_3(L) \qquad \frac{d\psi_2(L)}{dx} = \frac{d\psi_3(L)}{dx}$$

What are the conditions that are possible?

Penetration of Barrier 4

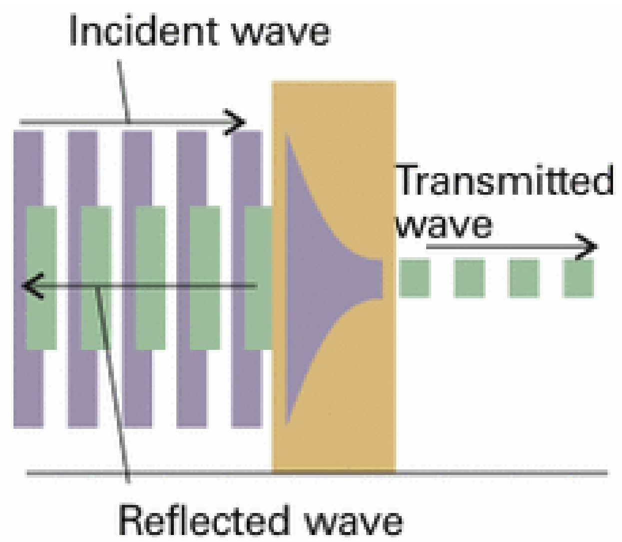
$$A + B = A' + B'$$

$$ikA - ikB = -\kappa A' + \kappa B'$$

$$A' Exp(-\kappa L) + B' Exp(\kappa L) = A'' Exp(ikL) + B'' Exp(-ikL)$$

$$-\kappa A' Exp(-\kappa L) + \kappa B' Exp(\kappa L) = ikA'' Exp(ikL) - ikB'' Exp(-ikL)$$

Now we assume that the initial state of the particle is approaching the barrier from the left B'' is zero



$$A + B = A' + B'$$

$$ikA - ikB = -\kappa A' + \kappa B'$$

$$A' Exp(-\kappa L) + B' Exp(\kappa L) = A'' Exp(ikL)$$

$$-\kappa A' Exp(-\kappa L) + \kappa B' Exp(\kappa L) = ikA'' Exp(ikL)$$

Penetration of Barrier 5

From the afore mentioned conditions show that

$$\frac{|A|^2}{|A''|^2} = \frac{1}{2} - \frac{1}{8}\left(\frac{\kappa}{k} - \frac{k}{\kappa}\right)^2 + \frac{1}{8}\left(\frac{\kappa}{k} + \frac{k}{\kappa}\right)^2 \cosh(2\kappa L)$$

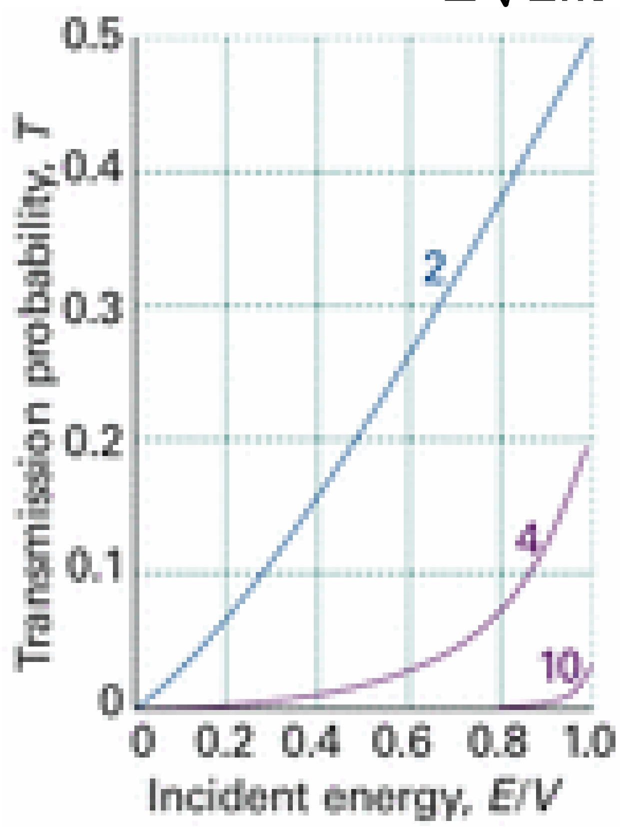
Transmission probability T is the ration of the probability travelling to right in zone 3 versus zone 1

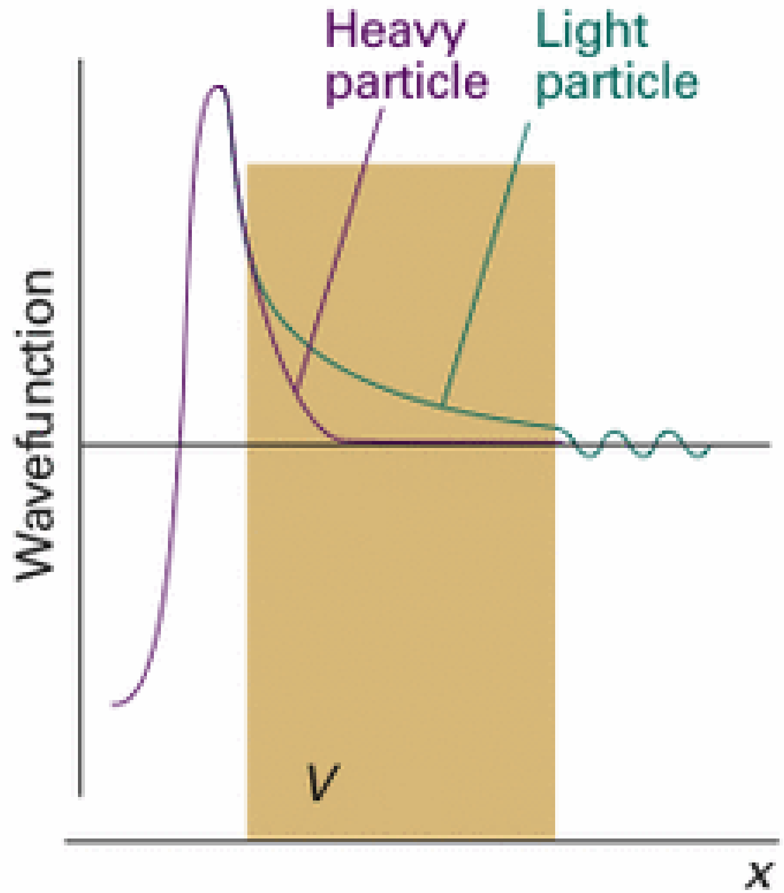
$$T = \frac{|A''|^2}{|A|^2} = \left[1 + \frac{\left(Exp(\kappa L) - Exp(-\kappa L)\right)^2}{16\frac{E}{V}\left(1 - \frac{E}{V}\right)}\right]^{-1}$$

For high, wide barriers (κL>>1) $\quad T \approx 16\frac{E}{V}\left(1 - \frac{E}{V}\right)Exp(-2\kappa L)$

Penetration of Barrier 6

Values are for $L\sqrt{2mV}\,/\,\eta$





For wide and large barriers transmision is small

Transmission probability decays with square root of mass

TUNNELING is important for light particles