Chapter 41 Quantum Mechanics

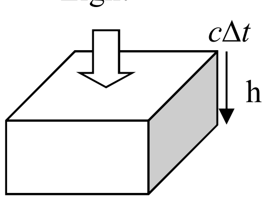
41.1 The Wave Function

From Wave Function to Particle Numers

Wave function of the plane wave of a EM wave:

$\vec{E}(x,t)=E_0\cos(kx-\omega t)\hat{j}$, $\vec{B}(x,t)=B_0\cos(kx-\omega t)\hat{k}$, propagating in the $\hat{i}$ direction

Energy density carried by the EM wave in vacuum is:



$$u_{EM}=\frac{E}{V}=\left\langle\frac{\varepsilon_0}{2}E_0^2\cos^2(kx-\omega t)+\frac{1}{2\mu_0}B_0^2\cos^2(kx-\omega t)\right\rangle$$

Since $B_0=E_0/C$, we obtain $u_{EM}(x,t)=\varepsilon_0 E_0^2\cos^2(kx-\omega t)$.

$$\langle u_{EM}(x,t)\rangle=\frac{1}{2}\varepsilon_0 E_0^2$$

Light intensity, I, is of the expression: $I=\frac{\text{Power}}{A}=\frac{Vu_{EM}}{A\Delta t}=\frac{hu_{EM}}{\Delta t}=cu_{EM}$.

We know from previous Chapter that the light is quantized and it is described as photons. If light intensity is described by photons, the relation will be:

$$\frac{N\times hf}{A\Delta t}=cu_{EM}=c\langle u_{EM}(x,t)\rangle=c\left\langle\varepsilon_0(E(x,t))^2\right\rangle \rightarrow N=\frac{V\varepsilon_0}{hf}\left\langle(E(x,t))^2\right\rangle$$

The number of photon is proportional to square of the electric field of the EM wave in which the wave function $\vec{E}(x,t)$ represents the wave nature of the EM wave.

The wave function describes the spatial and time behaviors of the photon while its square represents the finding probability or the number of the photon particle.

$$\frac{\mathrm{N}}{V}\propto\left\langle(\psi(x,t))^2\right\rangle \rightarrow \Delta N\propto\left\langle(\psi(x,t))^2\right\rangle\Delta V \rightarrow N\propto\int\left\langle(\psi(x,t))^2\right\rangle dV$$

The probability of finding the particle (the number of microscopic particles) is proportional to the square of the wave functions.

Motion of Particles Described by Waves

One particle wave function: $\Psi(x,y,z,t)=\Psi(\vec{r},t)\underset{time\_independent\_Schrodiger}{=}\psi(\vec{r})e^{-i\omega t}$, where

ω gives an information of the particle energy.

A system of many particles, the wave function description is:

$\Psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_N,t)=\psi(\vec{r}_1)\psi(\vec{r}_2)\cdots\psi(\vec{r}_N)e^{-i\omega t}$, where the parameter ω gives an information of total energy of the system.

Probability Density

One-dimensional case: $P(x)$ (probability per unit length), $\int P(x)dx=1$ or $\int P(x_i)dx=N$ when the number of particles is 1 or N. The wave function of one particle in one-dimensional motion shall satisfy the condition: $P(x)=|\Psi(x,t)|^2$. The unit of the wave function is $L^{-1/2}$.

Two-dimensional case: $P(x)$ (probability per unit area), $\int P(x,y)da=1$ or $\int P(x_i,y_i)da=N$ when the number of particles is 1 or N. The wave function of one particle in one-dimensional motion shall satisfy the condition:

$P(x)=|\Psi(x,y,t)|^2=|\Psi(\vec{r},t)|^2$. The unit of the wave function is L^{-1}.

Three-dimensional case: $P(x)$ (probability per unit volume), $\int P(x,y,z)da=1$ or $\int P(x_i,y_i,z_i)da=N$ when the number of particles is 1 or N. The wave function of one particle in one-dimensional motion shall satisfy the condition:

$P(x)=|\Psi(x,y,z,t)|^2=|\Psi(\vec{r},t)|^2$. The unit of the wave function is $L^{-3/2}$.

The wave function can be $\Psi(x,t)=\psi(x)e^{-i\omega t}$ or it can be $\Psi(x,t)=Ae^{ikx}e^{-i\omega t}$ for a free particle.

Physical Information from Waves

A free particle existing in one-dimensional space means that the probability to find it in the whole space is the 1, the number of this free particle.

$$\int_{-\infty}^{\infty} P(x)dx = 1 \rightarrow \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$

The probability of finding the particle in the arbitrary interval $a \le x \le b$:

$$\int_{a}^{b} |\Psi(x,t)|^2 dx = 1 \text{ for a time independent case} \rightarrow \int_{a}^{b} |\psi(x)|^2 dx = 1$$

How to find the physical information of the particle?

The probability to find the particle at x is $P(x)$ so the average position of the particle is

$$\int_{-\infty}^{\infty} xP(x)dx = \int_{-\infty}^{\infty} x|\Psi(x,t)|^2 dx = \int_{-\infty}^{\infty} x|\psi(x)|^2 dx = \int_{-\infty}^{\infty} x\psi^*(x)\psi(x)dx = \int_{-\infty}^{\infty} \psi^*(x)x\psi(x)dx$$

The average particle position is called an **expectation value.**
If the particle's property can be described by a function $f(x)$, the averaged property (expectation value of $f(x)$) of this particle is expressed as

$$\langle f(x)\rangle = \int_{-\infty}^{\infty} \psi^*(x)f(x)\psi(x)dx$$ The concept comes from statistics.

The wave function of the traveling light is $\vec{E}(x,t) = \hat{j}E_0 \sin(kx - \omega t)$ and we get used to the expression $\Psi(x,t) = A\sin(kx - \omega t)$ of the wave. We know that the probability function is a real spatial function while, in order to extend the space of the wave, the wave function can have an imaginary part.
We extend thus the space of the wave function to have a complex number:
$\Psi(x,t) = Ae^{i(kx-\omega t)} = A\cos(kx - \omega t) - iA\sin(kx - \omega t)$
While the probability function is still in real space:

$$P(x,t) = |\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t) = Ae^{-i(kx-\omega t)}Ae^{i(kx-\omega t)} = A^2$$

Can we get more information from the wave function?

$$-i\frac{\partial}{\partial x}A^{i(kx-\omega t)} = kA^{i(kx-\omega t)} = \frac{2\pi}{\lambda}A^{i(kx-\omega t)} = \frac{h}{\lambda}\frac{2\pi}{h}A^{i(kx-\omega t)} = \frac{p}{\hbar}A^{i(kx-\omega t)}$$

$$\rightarrow \; -i\hbar\frac{\partial}{\partial x}Ae^{i(kx-\omega t)} = pAe^{i(kx-\omega t)} \;\rightarrow\; p = -i\hbar\frac{\partial}{\partial x}$$

$$i\frac{\partial}{\partial t}A^{i(kx-\omega t)} = \omega A^{i(kx-\omega t)} = 2\pi f A^{i(kx-\omega t)} = \frac{2\pi}{h}hfA^{i(kx-\omega t)} = \frac{2\pi}{h}EA^{i(kx-\omega t)} = \frac{E}{\hbar}A^{i(kx-\omega t)}$$

$$\rightarrow \; i\hbar\frac{\partial}{\partial t}Ae^{i(kx-\omega t)} = EAe^{i(kx-\omega t)} \;\rightarrow\; E = i\hbar\frac{\partial}{\partial t}$$

Normalization

Example: Consider a wave function whose wave function is $\psi(x) = Ae^{-ax^2}$. (a) What is the value of A if this wave function is normalized?

$$\int_{-\infty}^{\infty}\left(Ae^{-ax^2}\right)\left(Ae^{-ax^2}\right)dx = 1 \;\rightarrow\; A^2\int_{-\infty}^{\infty}e^{-2ax^2}dx = 1 \;\rightarrow\; \frac{A^2}{\sqrt{2a}}\int_{-\infty}^{\infty}e^{-\left(\sqrt{2a}x\right)^2}d\sqrt{2a}x = 1$$

$$\frac{A^2}{\sqrt{2a}}\int_{-\infty}^{\infty}e^{-y^2}dy = 1$$

Since $\int_{-\infty}^{\infty}e^{-x^2}dx\int_{-\infty}^{\infty}e^{-y^2}dy = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-\left(x^2+y^2\right)}dxdy = \int_{0}^{\infty}\int_{0}^{2\pi}e^{-r^2}r\,d\theta dr = 2\pi\left[-\frac{1}{2}e^{-r^2}\right]_0^{\infty} = \pi$,

$$\rightarrow \; \int_{-\infty}^{\infty}e^{-y^2}dy = \sqrt{\pi} \;\rightarrow\; A = \left(\frac{2a}{\pi}\right)^{1/4}$$

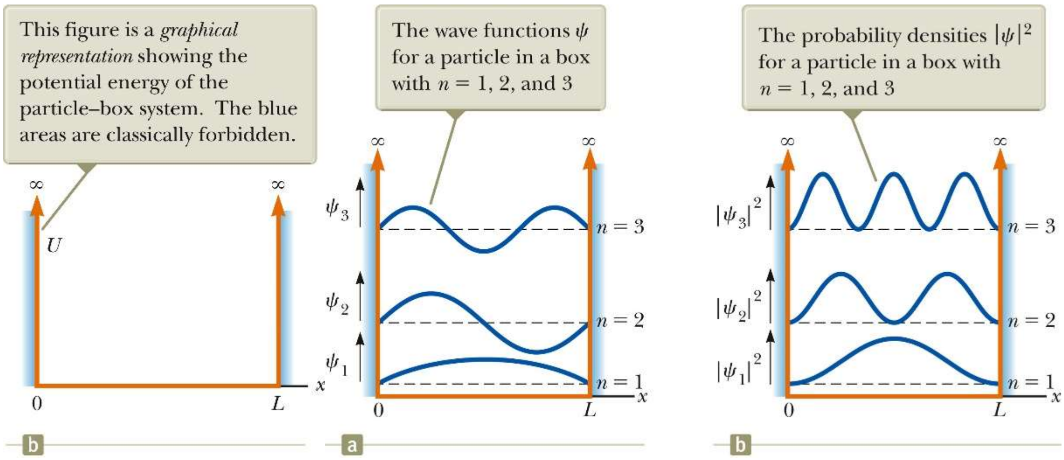
(b) What is the expectation value of x for this particle?

$$\psi(x) = Ae^{-ax^2} = \left(\frac{2a}{\pi}\right)^{1/4}e^{-ax^2}$$

$$\langle x\rangle = \int_{-\infty}^{\infty}\psi(x)x\psi(x)dx = \left(\frac{2a}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}xe^{-2ax^2}dx = 0$$

41.2 Quantum Particle Under Boundary Conditions

Quantized Particle



You may expect to find the quantized wave function of this particle from its boundary conditions.

Since $\psi(x)=0$ at $x=0$, we guess the wave function of $\psi(x)=A\sin(kx)$. In addition, the wave function shall satisfy the 2nd boundary condition of $\psi(x)=0$ at $x=L$. We therefore obtain the quantization condition

$$kL=n\pi \rightarrow k_nL=n\pi \rightarrow k_n=\frac{n\pi}{L}$$

The wave function can be written as $\psi_n(x)=A_n\sin\left(\frac{n\pi x}{L}\right)$.

Normalization: $\int_0^L\left(A_n\sin\left(\frac{n\pi x}{L}\right)\right)\left(A_n\sin\left(\frac{n\pi x}{L}\right)\right)dx=1 \rightarrow \psi_n(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$

The quantized energy is $E_n=\frac{\hbar^2k_n^2}{2m}=\frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$

The complete wave function shall be: $\Psi(x,t)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-i\omega t}$

$$\Psi(x,t)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-i\frac{E_n}{\hbar}t} \rightarrow \Psi(x,t)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-i\frac{\hbar}{2m}\left(\frac{n\pi}{L}\right)^2 t}$$

Expectation Value Exercise

What's the expectation value of the position x of the particle in the n^{th} quantum state?

$$\langle x\rangle = \int_{-\infty}^{\infty}\psi^*(x)x\psi(x)dx = \frac{2}{L}\int_0^L x\sin^2\left(\frac{n\pi x}{L}\right)dx$$

$$\langle x\rangle = \frac{2}{L}\int_0^L x\frac{1-\cos(2n\pi x/L)}{2}dx = \frac{2}{L}\left(\frac{L^2}{4}-\int_0^L \frac{x}{2}\frac{L}{2n\pi}d\left(\sin(2n\pi x/L)\right)\right)$$

$$\langle x\rangle = \frac{2}{L}\left(\frac{L^2}{4}-\left[\frac{x}{2}\frac{L}{2n\pi}\sin(2n\pi x/L)\right]_0^L+\int_0^L \sin(2n\pi x/L)\frac{L}{4n\pi}dx\right)=\frac{L}{2}$$

41.3 The Schrodinger Equation

Guess What's The Differential Equation for Deriving The Wave Function of a Microscopic Particle

The energy-momentum relation of the particle is $E = K + V = \frac{p^2}{2m} + V$.

Since the momentum corresponds to the spatial differential of the particle wave function:

$$p\Psi(x,t) = -i\hbar\frac{\partial}{\partial x}\Psi(x,t)$$

It means that you can extract the momentum information from the particle wave function.

The total energy corresponds to the time differential of the wave function:

$$E\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

You can extract the energy information of the particle from the wave function.

Rewrite the known energy conservation through the information extraction from the wave function:

$$E = \frac{p^2}{2m}+V \rightarrow E\Psi(x,t) = \frac{p^2}{2m}\Psi(x,t)+V\Psi(x,t) \rightarrow$$

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=\frac{(-i\hbar)^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)+V\Psi(x,t) \rightarrow$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)+V(x,t)\Psi(x,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$ (time dependent Schrodinger's eq)

If the potential is time independent

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)+V(x)\Psi(x,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

, the wave function could be separable $\Psi(x,t)=\psi(x)\phi(t)$, where

$$\frac{\partial}{\partial t}\Psi(x,t)=-i\omega\Psi(x,t)=-i\frac{E}{\hbar}\Psi(x,t) \rightarrow \frac{\partial}{\partial t}\phi(t)=-i\frac{E}{\hbar}\phi(t)$$

$$\rightarrow \phi(t)=e^{-i\frac{E}{\hbar}t}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)+V(x)\Psi(x,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

$$\rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)+V(x)\psi(x)=E\psi(x)$$

The Particle in a Box Revisited

Start from the Differential Equation – Write down the Schrodinger eq

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

Let $k=\frac{\sqrt{2mE}}{\hbar} \rightarrow \frac{d^2\psi(x)}{dx^2}+k^2\psi(x)=0 \rightarrow \psi(x)=A\sin(kx)+B\cos(kx)$

Take the boundary conditions into consideration:

$\psi(0)=0 \rightarrow B=0$

$\psi(L)=0 \rightarrow k_nL=n\pi \rightarrow \psi(x)=A\sin\left(\frac{n\pi x}{L}\right)$ & $E=\frac{\hbar^2}{2m}k^2=\frac{n^2\hbar^2\pi^2}{2mL^2}$

41.4 A Particle in a Well of Finite Height

Region I:

$x\le 0$, $\psi_I(x)=Ae^{\frac{\sqrt{2m(U-E)}}{\hbar}x}$

Region II:

$0\le x\le L$, $\psi_{II}(x)=Be^{i\frac{\sqrt{2mE}}{\hbar}x}+Ce^{-i\frac{\sqrt{2mE}}{\hbar}x}$

Region III:

$$L \le x\,,\quad \psi_{III}(x) = De^{-\frac{\sqrt{2m(U-E)}}{\hbar}x}$$

Continuous Condition:

At $x = 0$

$$\psi_I(0) = A = \psi_{II}(0) = B + C \;\rightarrow\; A = B + C$$

$$\left.\frac{d\psi_I(x)}{dx}\right|_{x=0} = \frac{\sqrt{2m(U-E)}}{\hbar}A = \left.\frac{d\psi_{II}(x)}{dx}\right|_{x=0} = i\frac{\sqrt{2mE}}{\hbar}(B-C) \rightarrow$$

$$\frac{\sqrt{2m(U-E)}}{\hbar}A = i\frac{\sqrt{2mE}}{\hbar}(B-C)$$

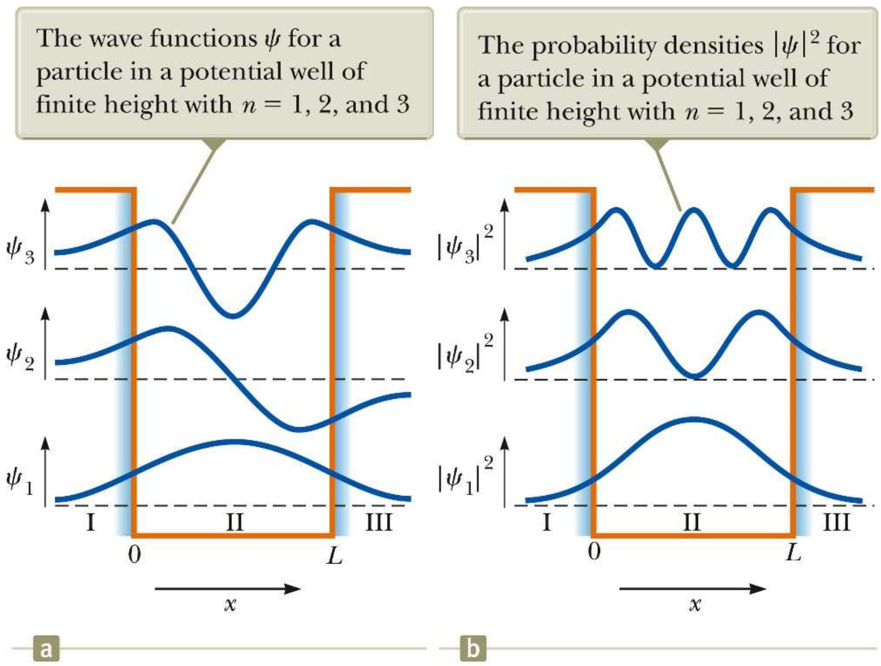
At $x = L$

$$\psi_{II}(L) = Be^{i\frac{\sqrt{2mE}}{\hbar}L} + Ce^{-i\frac{\sqrt{2mE}}{\hbar}L} = \psi_{III}(L) = De^{-\frac{\sqrt{2m(U-E)}}{\hbar}L} \;\rightarrow$$

$$Be^{i\frac{\sqrt{2mE}}{\hbar}L} + Ce^{-i\frac{\sqrt{2mE}}{\hbar}L} = De^{-\frac{\sqrt{2m(U-E)}}{\hbar}L}$$

$$\left.\frac{d\psi_{II}(x)}{dx}\right|_{x=L} = \left.\frac{d\psi_{III}(x)}{dx}\right|_{x=L} \rightarrow$$

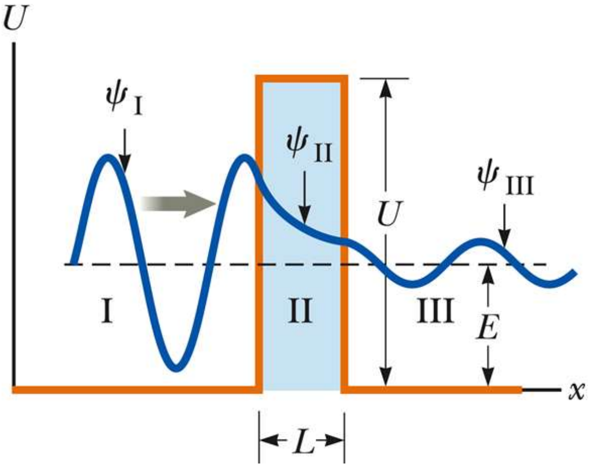
$$i\frac{\sqrt{2mE}}{\hbar}\left(Be^{i\frac{\sqrt{2mE}}{\hbar}L} - Ce^{-i\frac{\sqrt{2mE}}{\hbar}L}\right) = -\frac{\sqrt{2m(U-E)}}{\hbar}De^{-\frac{\sqrt{2m(U-E)}}{\hbar}L}$$



41.5 Tunneling Through a Potential Energy Barrier

Region I: $x \le 0$, $\psi_I(x) = Ae^{ik_I x} + Be^{-ik_I x}$
Region II: $0 \le x \le L$, $\psi_{II}(x) = Ce^{k_{II} x} + De^{-k_{II} x}$
Region III: $L \le x$, $\psi_{III}(x) = Ee^{ik_I x}$

$$A + B = C + D \quad (1)$$
$$ik_I(A - B) = k_{II}(C - D) \quad (2)$$
$$Ce^{k_{II}L} + De^{-k_{II}L} = Ee^{ik_I L} \quad (3)$$
$$k_{II}\left(Ce^{k_{II}L} - De^{-k_{II}L}\right) = ik_I Ee^{ik_I L} \quad (4)$$



In Region II, the wave function is $\psi(x) = Ae^{-k_{II}x} = Ae^{-\frac{\sqrt{2m(U-E)}}{\hbar}x}$

Assume that the barrier is located from $x = 0$ to $x = L$.

The transmission probability is $P \propto |\psi(x)|^2$, thus

$$T \approx e^{-2k_{II}L} = e^{-2\frac{\sqrt{2m(U-E)}}{\hbar}L}$$

Example: An electron is incident on a square barrier of height 5 eV.

(a) What is the probability that the electron tunnels through the barrier with a width of 1.0 nm?

$$k = \frac{\sqrt{2mU}}{\hbar} = \frac{\sqrt{2 \times 9.11 \times 10^{-31} \times 5 \times 1.602 \times 10^{-19}}}{6.626 \times 10^{-34} / 2\pi} = 1.15 \times 10^{10}$$
$$T \approx e^{-2kL} = e^{-23} = 1 \times 10^{-10}$$

(b) If the current flow across the barrier with zero barrier height is $I_0 = 1$ A, what will the final current for the barrier height of 5 eV with a width of 1.0 nm?

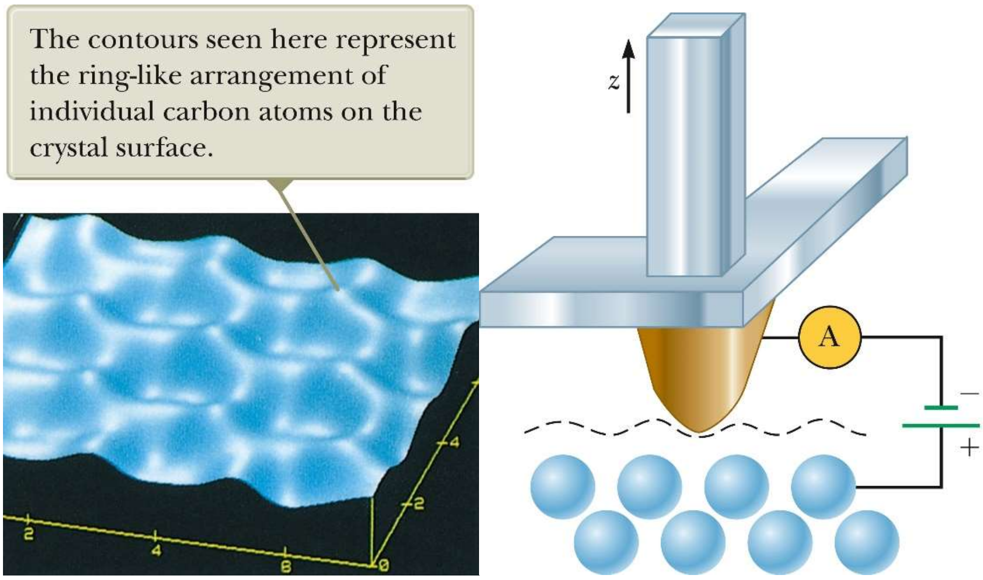
$I \approx I_0 T = 0.1 \ \ \text{(nA)}$

(c) What is the probability for the barrier width of 0.1 nm?

$T \approx e^{-2kL} = e^{-2.3} = 0.1$, For every one angstrom, the tunneling current decay to one tenth.

41.6 Application of Tunneling

Scanning Tunneling Microscope



41.7 The Simple Harmonic Oscillator

The potential energy of the simple harmonic oscillator:

$$U = \frac{kx^2}{2}, \quad \omega = \sqrt{\frac{k}{m}} \rightarrow U = \frac{m\omega^2 x^2}{2}$$

Schrodinger's Eq:

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

Guess solution: $\psi(x) = Ae^{-Bx^2}$

$$-\frac{\hbar^2}{2m}A\left(-2B + 4B^2x^2\right)e^{-Bx^2} + \frac{m\omega^2}{2}x^2 Ae^{-Bx^2} = EAe^{-Bx^2}$$

$$-\frac{\hbar^2}{2m}\left(-2B+4B^2x^2\right)+\frac{m\omega^2}{2}x^2=E$$

$$\frac{4\hbar^2B^2}{m}=m\omega^2\,,\quad B=\frac{m\omega}{2\hbar}$$

$$E=\frac{\hbar^2B}{m}=\frac{1}{2}\hbar\omega$$

→ $\psi(x)=Ae^{-\frac{m\omega x^2}{2\hbar}}$

Generalized results: $E_0=\frac{1}{2}\hbar\omega\,,\ \psi_0(x)=A_0e^{-\frac{m\omega x^2}{2\hbar}}$

$$E_n=\left(n+\frac{1}{2}\right)\hbar\omega\,,\quad \Delta E=E_{n+1}-E_n=\hbar\omega$$