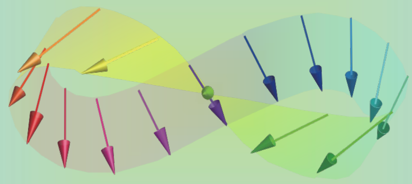
Nanoelectronics
06



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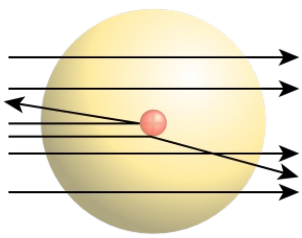
12:00 Thursday, 02/February/2023 (P/T 005A)

Quick Review over the Last Lecture

( ) model :



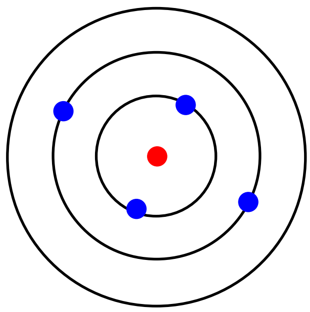
But suffers from a limitation :

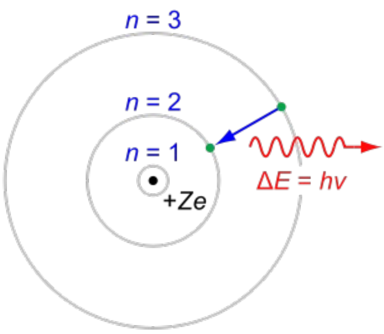
( ) levels

( ) principle :

( )

( ) model :





Experimental proof :

( ) series

Contents of Nanoelectonics

06 Schrödinger Equation

- Schrödinger equation
- Particle position
- Hermite operator
- 1D trapped particle

Schrödinger Equation

In order to express the de Broglie wave, Schrödinger equation is introduced in 1926 :

$$\frac{\hbar^2}{2m}\nabla^2\psi + (E - V)\psi = 0 \qquad \left(\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

E : energy eigen value and ψ : wave function

Wave function represents probability of the presence of a particle $|\psi|^2 = \psi^*\psi$

ψ^* : complex conjugate (*e.g.*, $z = x + iy$ and $z^* = x - iy$)

Propagation of the probability (flow of wave packet) :

$$\boldsymbol{j} = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$$

Operation = observation :

$$-\frac{\hbar^2}{2m}\nabla^2\psi = (E - V)\psi$$

$$-i\hbar\frac{\partial}{\partial t}\psi = H\psi$$

Complex Conjugates in the Schrödinger Equation

In the Schrödinger equation, 1D wave propagating along x-direction is expressed as

$$\psi_+ = A\sin\left\{2\pi\left(\frac{x}{\lambda} - vt\right) + \alpha\right\}$$

For the wave along -x-direction,

$$\psi_- = B\sin\left\{2\pi\left(\frac{x}{\lambda} - vt\right) + \beta\right\}$$

At $t = 0$,

$$\psi = A\sin\left(2\pi\frac{x}{\lambda} + \alpha\right) + B\sin\left(-2\pi\frac{x}{\lambda} + \beta\right)$$

For $B = -A$ and $\alpha = -\beta$, these waves .

On the other hand, waves with complex conjugates :

$$\psi = A\sin\left\{2\pi i\left(\frac{x}{\lambda} - vt\right) + \alpha\right\} + B\sin\left\{2\pi i\left(\frac{x}{\lambda} - vt\right) + \beta\right\}$$

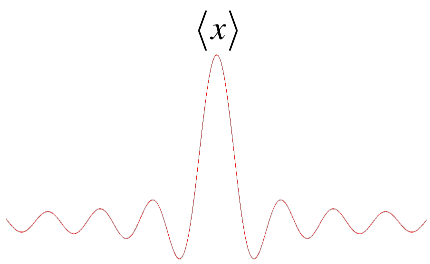
At $t = 0$,

$$\psi = A\sin\left(2\pi i\frac{x}{\lambda} + \alpha\right) + B\sin\left(-2\pi i\frac{x}{\lambda} + \beta\right)$$

→ contains - information

Position of a Particle

In the Schrödinger equation, the meaning of a particle position $\langle x \rangle$ is :



Expectation = Expected numbers × Probability

$$\langle x \rangle = \int x \times \psi^*(x)\psi(x)dx = \int \psi^*(x)x\psi(x)dx$$

Standard deviation :

$$\left\langle \left(x - \langle x \rangle\right)^2 \right\rangle = \left\langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \right\rangle$$

$$= \langle x \rangle^2 - 2\langle x \rangle\langle x \rangle + \langle x \rangle^2 = \langle x^2 \rangle - \langle x \rangle^2$$

Expectation of a momentum $-i\hbar \frac{\partial}{\partial x}$:

$$\langle p \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right)\psi dx$$

Eigen value and eigen function :

If a function stays the same after applying an operator, for example,

$$-i\hbar \frac{\partial}{\partial x} e^{inx} = \hbar n e^{inx}$$

Eigen value :

Eigen function :

Hermite Operator

Assuming a Hamiltonian satisfies :

$$\int \left(H\psi(x,t)\right)^* \psi(x,t)dx = \int \psi^*(x,t)H\psi(x,t)dx$$

$\rightarrow H$: Hermite operator

By using this assumption,

$$\frac{d}{dt}\int dx\psi^*(x,t)x\psi(x,t) = \frac{1}{i\hbar}\int dx\psi^*(x,t)(xH - Hx)\psi(x,t) \qquad -i\hbar\frac{\partial}{\partial t}\psi = H\psi$$

Here, $xH - Hx \neq 0$

Communication relation : [A,B] = AB - BA

Bra-ket Notation

Paul A. M. Dirac invented a notation based on Heisenberg-Born's matrix analysis :

A wave function consists of a complex vector :

$$\psi(x) = g(x) + ih(x)$$

Here, $\begin{cases} g(x) = (g_0, g_1, g_2, \cdots, g_n, \cdots) \\ h(x) = (h_0, h_1, h_2, \cdots, h_n, \cdots) \end{cases}$

By assuming $a_n = g_n + ih_n$, a ket vector is defined as $|\psi\rangle = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix}$

In order to calculate a probability, $\int \psi^*(x)\psi(x)dx$

$$\begin{cases} \psi(x) = a_0\phi_0(x) + a_1\phi_1(x) + a_2\phi_2(x) + \cdots + a_n\phi_n(x) + \cdots \\ \psi^*(x) = a_0{}^*\phi_0(x) + a_1{}^*\phi_1(x) + a_2{}^*\phi_2(x) + \cdots + a_n{}^*\phi_n(x) + \cdots \end{cases}$$

$$\int \psi^*(x)\psi(x)dx = a_0{}^*a_0 + a_1{}^*a_1 + a_2{}^*a_2 + \cdots + a_n{}^*a_n + \cdots$$

$$\therefore \int \psi^*(x)\psi(x)dx = \begin{pmatrix} a_0{}^* & a_1{}^* & a_2{}^* & \cdots & a_n{}^* & \cdots \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix} = \langle\psi|\psi\rangle$$

* http://www.wikipedia.org/

Bra-ket Notation (Cont'd)

A bra vector is defined as

$$\langle\psi| = \begin{pmatrix} a_0{}^* & a_1{}^* & a_2{}^* & \cdots & a_n{}^* & \cdots \end{pmatrix}$$

Therefore, an inner product is written as

$$\int f^*(x)g(x)dx = \langle f|g\rangle$$

This bra-ket notation satisfies

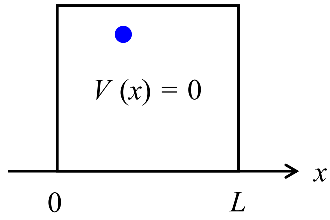
$$\langle f|g\rangle = \langle g|f\rangle^*$$

$\rightarrow$ bra + ket =

1D Trapped Particle

In 1D space, a free particle motion is expressed by the Schrödinger equation :

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



For a time-independent case, $\psi(x) = e^{\lambda x}$ can be assumed.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}e^{\lambda x} = Ee^{\lambda x} \qquad \therefore -\frac{\hbar^2}{2m}\lambda^2 e^{\lambda x} = Ee^{\lambda x}$$

By using $k = \frac{\sqrt{2mE}}{\hbar}$,

Since the particle is trapped in $0 \le x \le L$, $\psi =$ outside of this region.

Boundary conditions : $\psi(0) = \psi(L) =$.

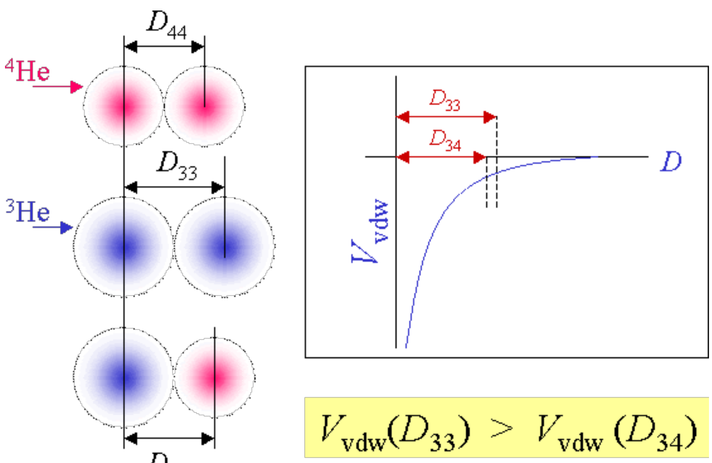
1D Trapped Particle - Zero-point motion

According to the Schrödinger equation, energy is defined as

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad (n = 1,2,3,\ldots)$$

Even for the minimum eigen energy with $n = 1$,

→



* http://www.sci.osaka-cu.ac.jp/phys/ult/invitation/cryo/mixture.html

1D Trapped Particle (Cont'd)

Therefore, the wave function is written as

$$\psi_n(x) = 2Ai\sin\left(\frac{n\pi}{L}x\right) =$$

In order to satisfy the normalisation : $\int \psi^* \psi dx = 1$

$$\int_0^L \psi^* \psi dx = \int_0^L C^2 \sin^2\left(\frac{n\pi}{L}x\right) dx$$

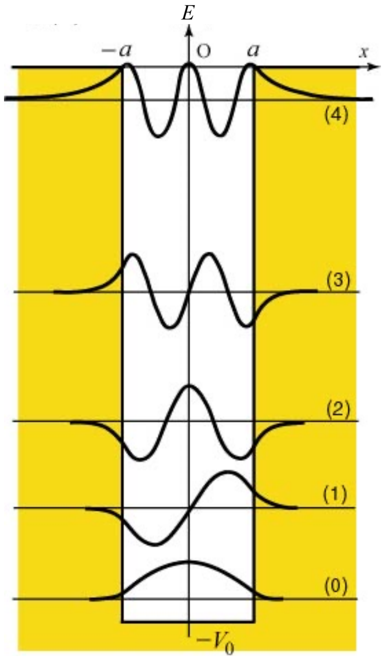
$$=$$

$$\therefore \quad = 1$$

$$\therefore$$

Finally, the wave function is obtained as

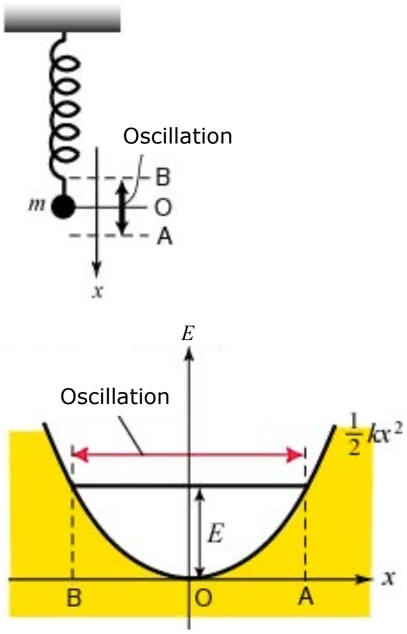
$$\psi_n(x) =$$



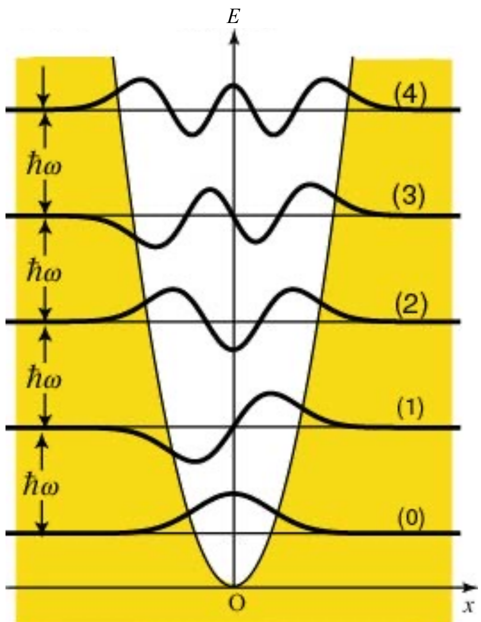
* http://www2.kutl.kyushu-u.ac.jp/seminar/MicroWorld2/2Part3/2P31/energy_eigenvalue.htm

1D Harmonic Oscillator

A crystalline lattice can be treated as a harmonic oscillator :



→ Phonon oscillation



* http://www.kutl.kyushu-u.ac.jp/seminar/MicroWorld2/2Part1/2P16/tunnel_effect.htm