Nanoelectronics

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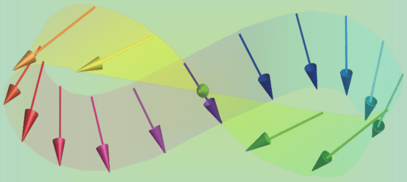

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Quick Review over the Last Lecture

Major surface analysis methods :

Techniques	Probe	Signals	Composition	Structure	Electronic state
Scanning tunneling microscopy (STM)				• Metallic surface morphology • Atom manipulation	
Atomic force microscopy (AFM)				• Surface morphology • Surface friction • Magnetic stray field	
Transmission electron microscopy (TEM)				• Atomic cross-section • Diffraction patterns (t < 30 nm)	
Scanning electron microscopy (SEM)			• Energy dispersive X-ray analysis (EDX) • X-ray photoelectron spectroscopy (XPS) • Secondary ion mass spectroscopy (SIMS)	• Atomic surface morphology • Low energy electron diffraction (LEED)	• EDX • XPS

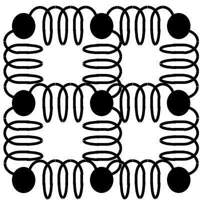
Contents of Nanoelectonics

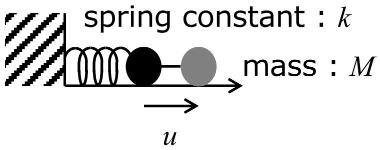
10 Harmonic Oscillator

- 1D harmonic oscillator
- 1D periodic potential
- Brillouin zone

Harmonic Oscillator

Lattice vibration in a crystal :





Hooke's law :

$$M\frac{d^2u}{dt^2} = -ku$$

Here, we define

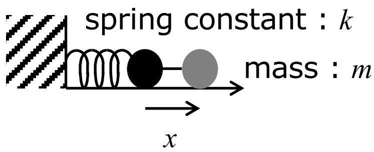
$$\omega = \sqrt{\frac{k}{M}} \qquad \therefore \frac{d^2u}{dt^2} = -\omega^2 u$$

$\rightarrow$

1D Harmonic Oscillator

For a 1D harmonic oscillator, Hamiltonian can be described as :

$H =$



Here, $k = m\omega^2$.

By substituting this to the Schrödinger equation,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\psi(x) = E\psi(x)$$

Here, for $x \rightarrow$, $\psi \rightarrow$.

By substituting x with $\alpha\xi$ (α : a dimension of length and ξ : dimensionless)

$$\left(-\frac{\hbar^2}{2m\alpha^2}\frac{d^2}{d\xi^2} + \frac{1}{2}m\omega^2\alpha^2\xi^2\right)\psi(x) = E\psi(x) \qquad \left(\frac{d}{dx} = \frac{1}{\alpha}\frac{d}{d\xi}\right)$$

By dividing both sides by $\hbar\omega$ in order to make dimensionless,

$$\left(-\frac{\hbar}{2m\omega\alpha^2}\frac{d^2}{d\xi^2} + \frac{m\omega\alpha^2}{2\hbar}\xi^2\right)\psi(x) = \frac{E}{\hbar\omega}\psi(x)$$

Simplify this equation by defining

1D Harmonic Oscillator (Cont'd)

$$\left(-\frac{1}{2}\frac{d^2}{d\xi^2}+\frac{1}{2}\xi^2\right)\psi(x)=\frac{\lambda}{2}\psi(x)$$

$$\therefore \frac{d^2}{d\xi^2}\psi(x)=(\xi^2-\lambda)\psi(x)$$

For $|\xi| \to \infty$, $\frac{d^2}{d\xi^2}\psi(x)=\xi^2\psi(x)$.

$$\psi(x)=A\exp\left(-\frac{1}{2}\xi^2\right) \qquad E=\frac{1}{2}\hbar\omega$$ (lowest eigen energy)(zero-point energy)

In general,

$$\psi(x)=H(\xi)\exp\left(-\frac{1}{2}\xi^2\right)$$

By substituting this result into the above original equation,

$$\frac{d^2}{d\xi^2}\left\{H(\xi)\exp\left(-\frac{1}{2}\xi^2\right)\right\}=(\xi^2-\lambda)H(\xi)\exp\left(-\frac{1}{2}\xi^2\right)$$

$$\therefore \frac{d^2H^2(\xi)}{d\xi^2}-2\xi\frac{dH(\xi)}{d\xi}-(\lambda-1)H(\xi)=0$$

= Hermite equation by classical dynamics

1D Periodic Potential

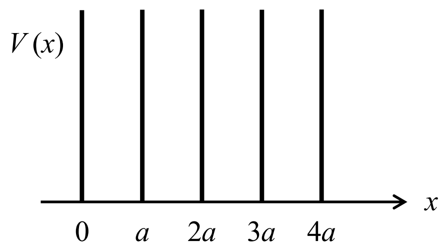
In a periodic potential energy *V* (*x*) at *na* (*n* = 1,2,3,…),

$$\psi\,(x+a)=\exp(iKa)\psi(x)$$

K : constant (phase shift : *Ka*)

A potential can be defined as

$$V(x=na)=V_0\delta(x-na)$$



The corresponding Schrödinger equation for a particle with a mass of *m* and an energy of *E* can be defined as

$$\begin{cases}-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)= & [\,x=na, \quad n=0,1,2,\cdots] \\ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)= & [na<x<(n+1)a, \quad n=0,1,2,\cdots]\end{cases}$$

Assuming the following general solution in the region $0 \le x < a$,

$$\psi(x)=A\exp(ikx)+B\exp(-ikx) \qquad (1)$$

where A, B and k are constants. By substituting $\psi(x)$ to the above Schrödinger equation, $k=$.

At $x=na$, $k'=\frac{\sqrt{2m\{V(x)-E\}}}{\hbar}=K-k=$.

For the neighbouring region $a \leq x < 2a$,

$$\psi(x) = \exp(iKa)\psi(x-a) = \exp(iKa)[A\exp\{ik(x-a)\} + B\exp\{-ik(x-a)\}] \quad (2)$$

Therefore, for $na \leq x < (n+1)a$, using $\tilde{x} = x - na$ $(0 < \tilde{x} < a)$,

$$\psi(x) = \psi(\tilde{x} + na) = \{\exp(iKa)\}^n \psi(\tilde{x}) = \exp(inKa)\{A\exp(ik\tilde{x}) + B\exp(-ik\tilde{x})\}$$

By taking $x \to a$ for Eqs. (1) and (2), boundary conditions are the continuity of $\psi(a)$ and $\psi'(a)$,

$$\psi(a)\text{: } A\exp(ika) + B\exp(-ika) = \exp(iKa)(A+B) \quad [\because \exp\{\pm ik(x-a)\} \to 1].$$

$$\therefore \qquad = 0 \qquad (3)$$

$$\psi'(a)\text{: } ik\exp(iKa)(A-B) - ik\{A\exp(ika) - B\exp(-ika)\} = \frac{2nV_0}{\hbar^2}\{A\exp(ika) + B\exp(-ika)\}$$

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

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

$$\therefore \lim_{x\to a}\left\{\frac{d}{dx}\psi(x) - \frac{d}{dx}\psi(-x)\right\} = -\frac{2mV_0}{\hbar^2}\psi(a)$$

This is a phase shift between the wave functions between the regions $0 < x < a$ and $a \leq x < 2a$].

$$\therefore A\left\{\left(-1 - \frac{2nV_0}{ik\hbar^2}\right)\exp(ika) + \exp(iKa)\right\} + B\left\{\left(1 - \frac{2nV_0}{ik\hbar^2}\right)\exp(ika) - \exp(iKa)\right\} = 0 \qquad (4)$$

By formulating matrix to combine these two boundary conditions (3) and (4),

$$\begin{pmatrix} \exp(ika) - \exp(iKa) & \exp(-ika) - \exp(iKa) \\ \left(-1 - \frac{2nV_0}{ik\hbar^2}\right)\exp(ika) + \exp(iKa) & \left(1 - \frac{2nV_0}{ik\hbar^2}\right)\exp(-ika) - \exp(iKa) \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = 0$$

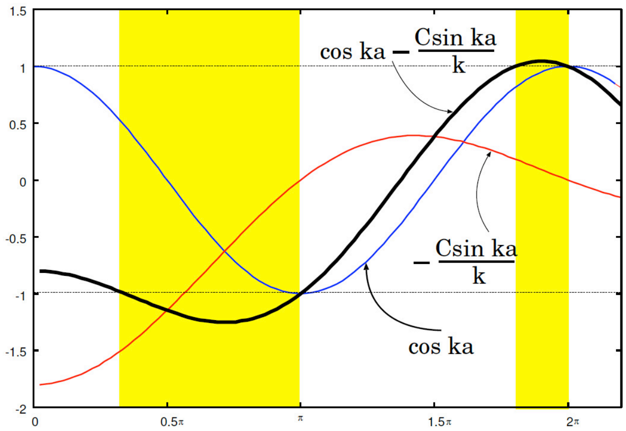
In order to obtain *A* and *B* (≠ 0), the determinant of the matrix should be 0.

$$\{\exp(ika) - \exp(iKa)\}\left\{\left(1 - \frac{2nV_0}{ik\hbar^2}\right)\exp(-ika) - \exp(iKa)\right\}$$
$$- \{\exp(-ika) - \exp(iKa)\}\left\{\left(-1 - \frac{2nV_0}{ik\hbar^2}\right)\exp(ika) + \exp(iKa)\right\} = 0$$

$\therefore$

1D Periodic Potential (Cont'd)

Now, the answers can be plotted as



In the yellow regions,

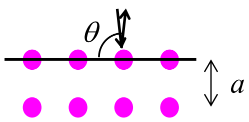
→ .

→ ( )

* http://homepage3.nifty.com/iromono/kougi/index.html

Brillouin Zone

Bragg's law : $n\lambda = 2d\sin\theta$



For $\theta \sim 90°$ $(\pi / 2)$,

$n\lambda \approx 2a$ → reflection

Therefore, no travelling wave for

$$k = \frac{2\pi}{\lambda} = \frac{n\pi}{a} \qquad n = 1, 2, 3, \ldots$$

→

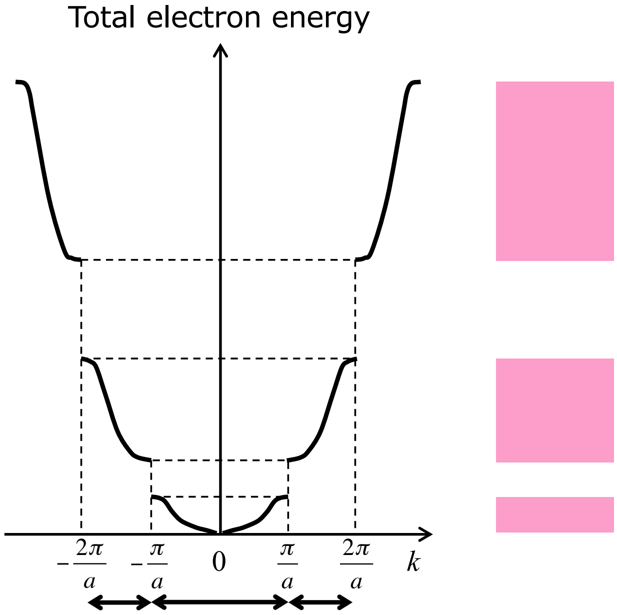
Allowed band :

$\leq k \leq$

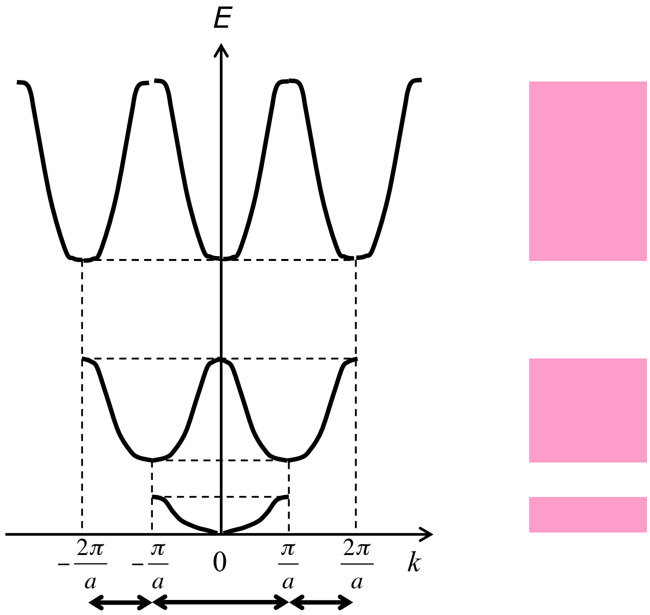
→

In general, bands are

$$k = \frac{2\pi}{\lambda} = \frac{n\pi}{d\sin\theta} \equiv k_n \qquad n = 1, 2, 3, \ldots$$



Periodic Potential in a Crystal



Energy band diagram

(zone)

↔   zone