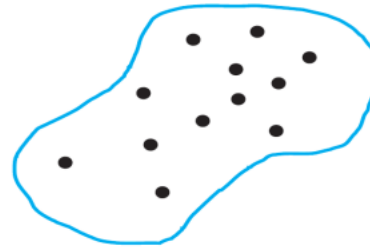


ECE320 RC1

Solid-types

Solids :

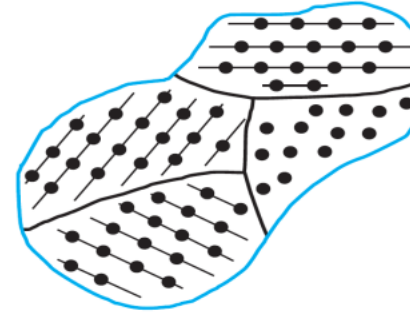
- Amorphous



(a)

All atoms or ions are periodically ranged in a short range (a few atoms)

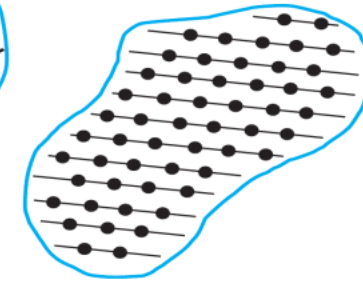
- Polycrystals



(b)

Multiple crystalline grains randomly packed

- Single crystals



(c)

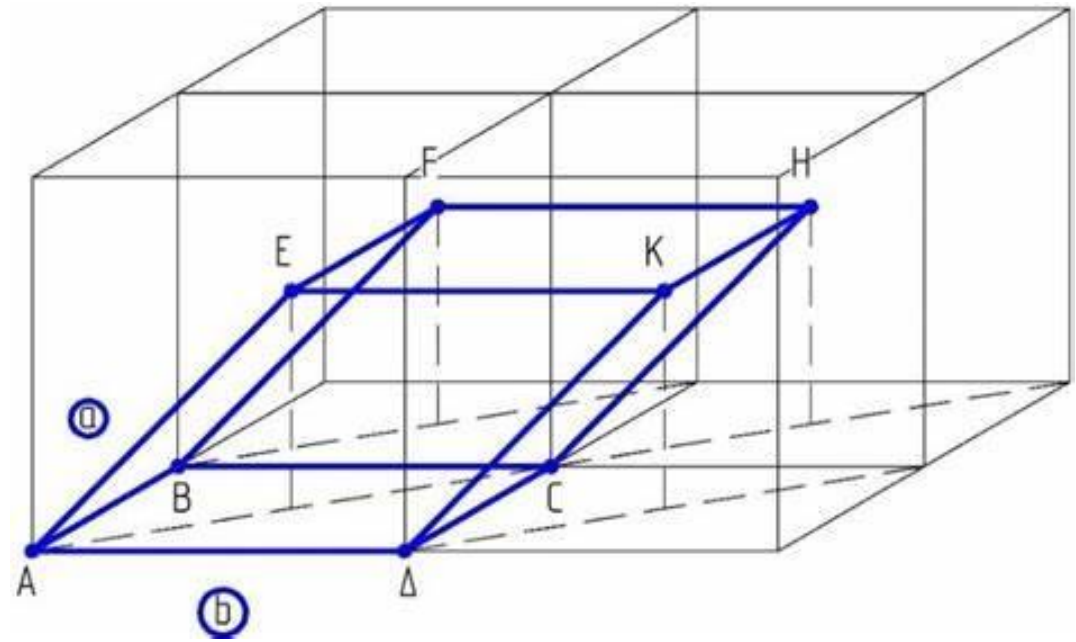
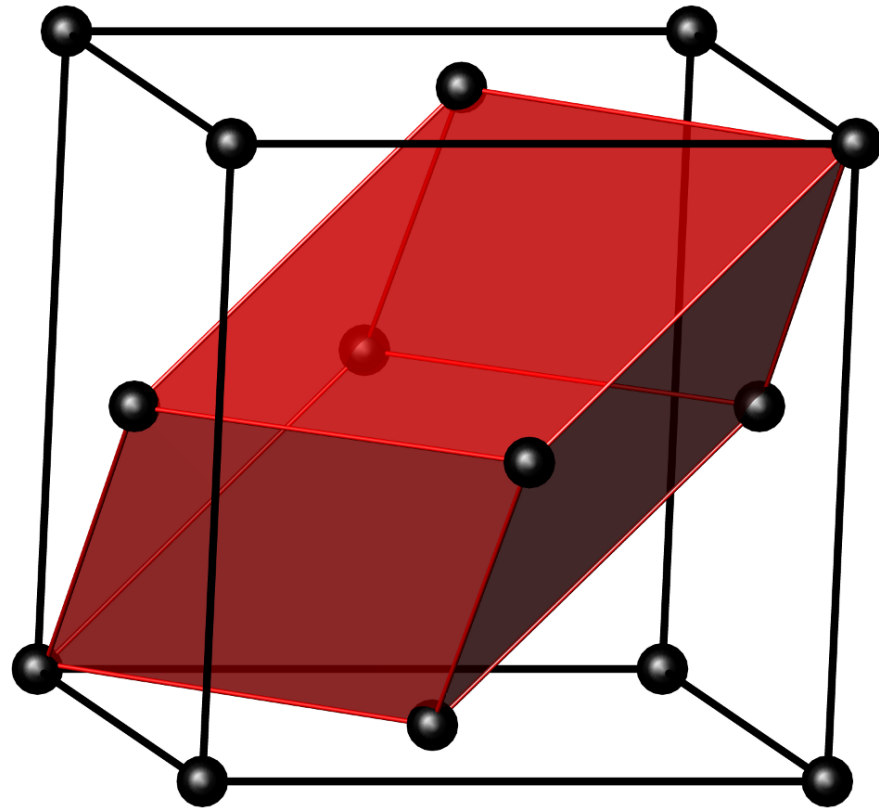
All atoms or ions are periodically ranged in a long range (μm scale)

Characteristics of Crystals

- Specific shape and fixed melting point
- Atoms or ions periodically arranged in a relatively large scale (μm)

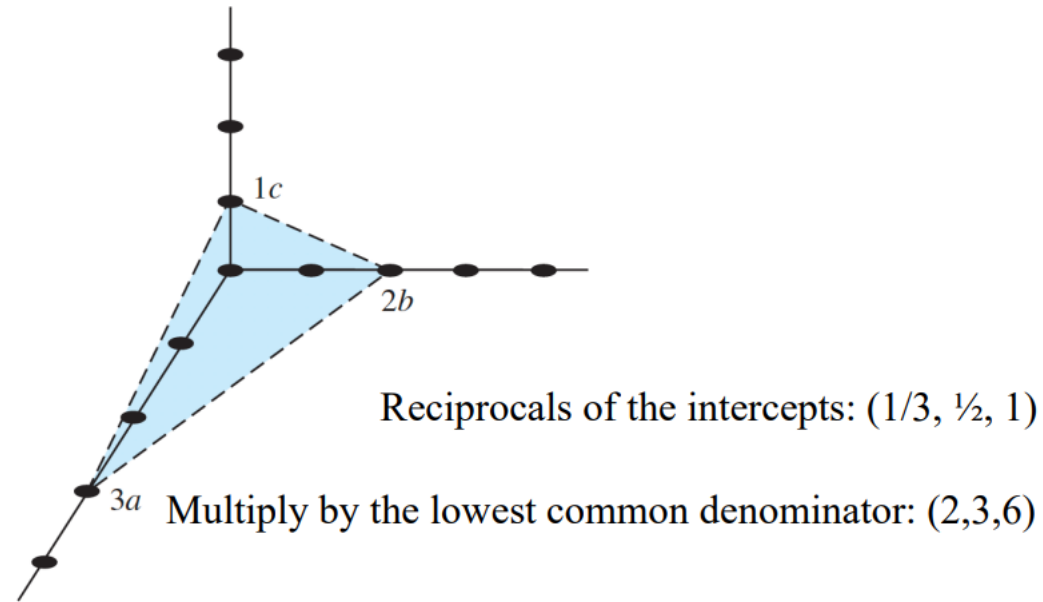
All semiconductors covered in this course are assumed to be single crystalline.

Solid-primitive cell and unit cell



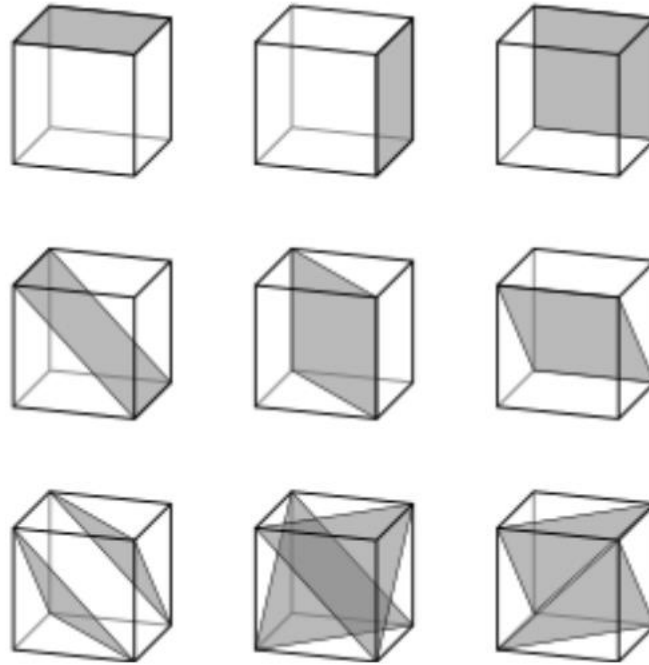
Solid-how to describe a plane-miller index

Crystalline Plane and Miller Index



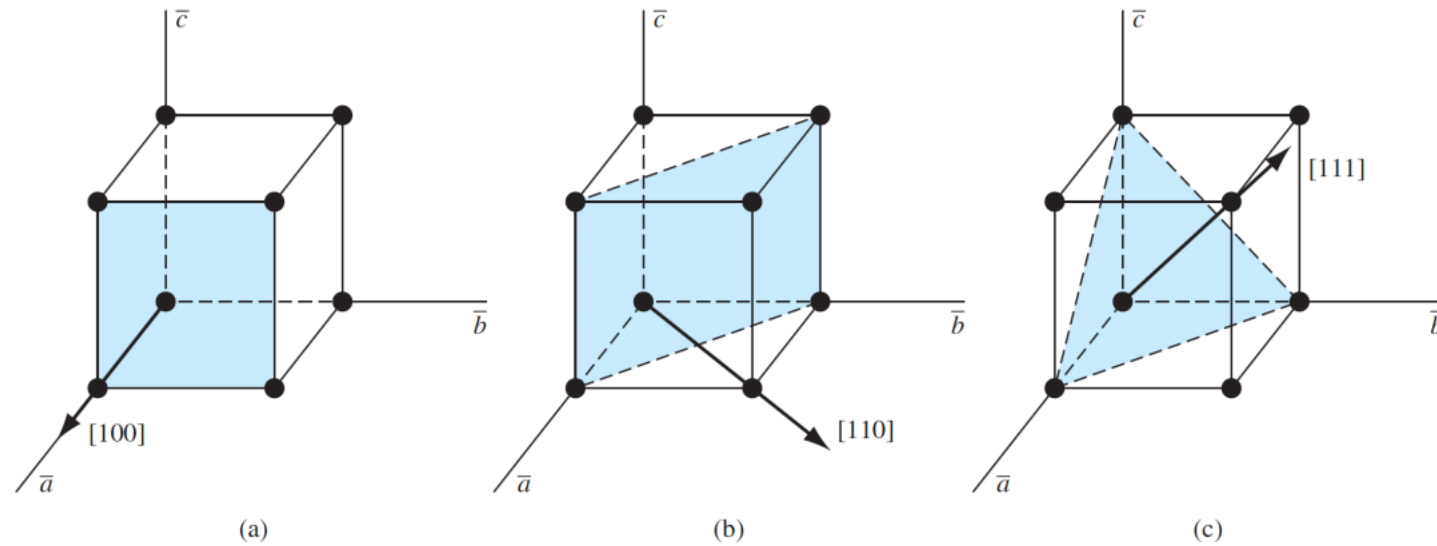
Solid-how to describe a plane-miller index

Identify crystalline plane



Solid-how to describe a direction

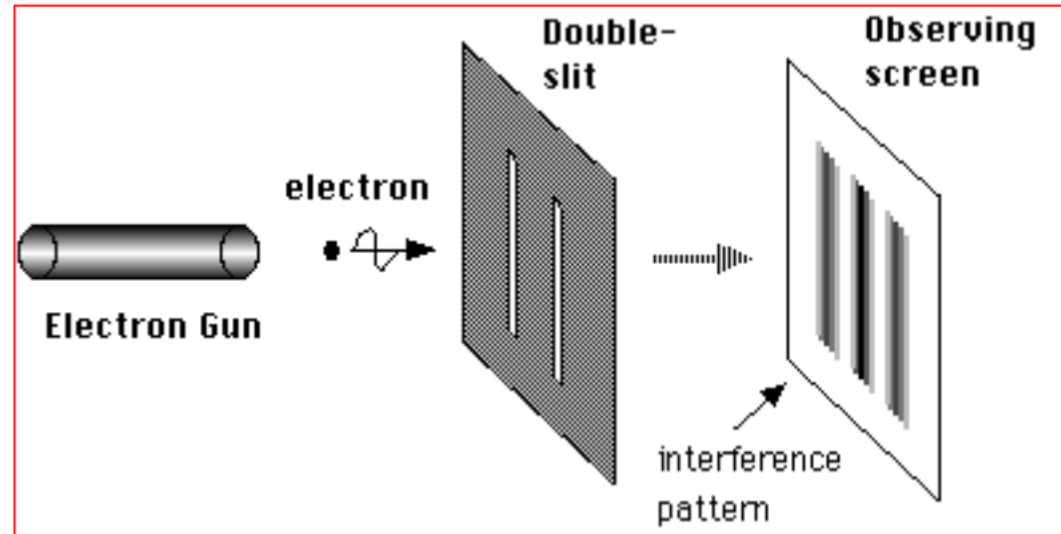
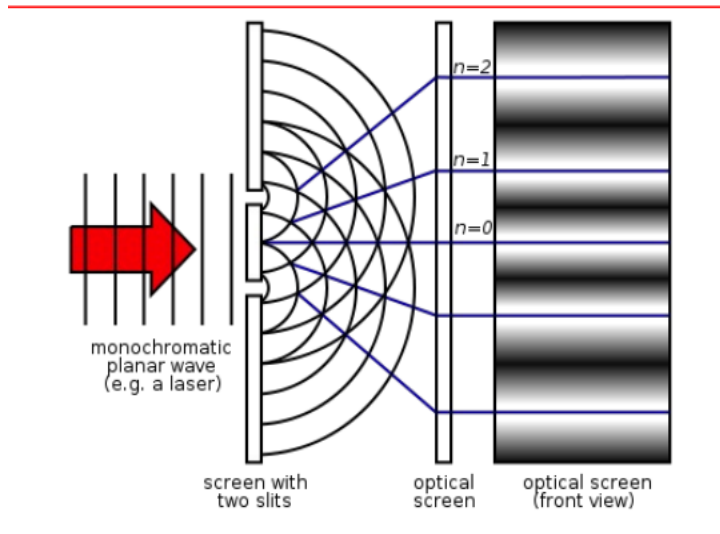
Directions in Crystals



In cubic lattice: $[hkl]$ direction is perpendicular to the (hkl) plane

QM-why we need it-electron wave

- In class: double-slit interference experiment can be done by sending a single electron or photon at one time



[Dr Quantum Double Slit Experiment \(youtube.com\)](https://www.youtube.com/watch?v=DrQuantumDoubleSlitExperiment)

QM-why we need it-photon particle

- In class: photon-electric effect

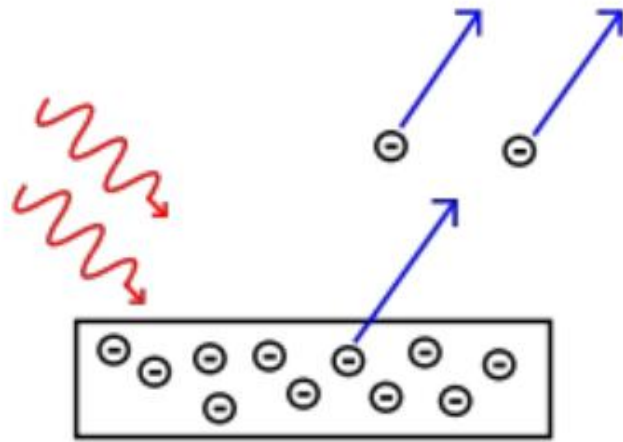
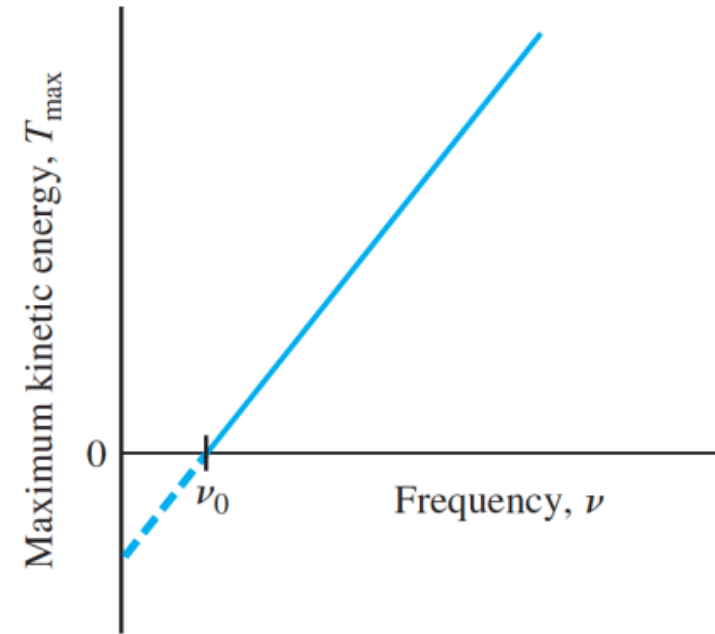


Photo-electric experiment



QM-why we need it-other stuff

- Radioactivity
- Stability of atom
- Hydrogen spectrum
- Blackbody radiation
- Compton scattering
-

QM—we need a new way to describe these behaviors

- If experiments don't say so, why should we believe the ridiculous quantum mechanics?
- The point is that if we follow the arguments of QM, we can explain the results of those experiments.
- We can also use it to build useful things. This semiconductor course is a really good example.
- We can also use it to make predictions and those predictions are verified by new experiments.
- So far, quantum mechanics is true.

QM-how to describe electron

- Probability wave
- You can view it as a three-dimension complex number field
- The square of the modulus of the complex number represents the probability density to find an electron at a given place
- If you think of the electric field wave,

Light = electromagnetic wave $\vec{\mathcal{E}}(x, t) = \vec{\mathcal{E}}_0 \sin \left[2\pi \left(\frac{x}{\lambda} - \frac{t}{T} \right) \right]$

Light intensity $I \propto \left| \vec{\mathcal{E}} \right|^2$

$\rightarrow \left| \vec{\mathcal{E}} \right|^2$ is a measure of the probability of finding a photon

QM-how to describe electron

Normalizable:

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

In 1924, Louis de Broglie hypothesized in his Ph.D. thesis that matter also has wave properties. He postulated that matter particles, like photons, have a wavelength called the de Broglie wavelength, is given by:

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$

where the momentum, p , is determined by the kinetic energy ($E = p^2/2m$).

QM-Schrodinger's equation

- Time-dependent

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

In-class exercise: try plugging in the following plane-wave solution into Schrödinger's equation:

$$\Psi(x, t) = A \exp[i(kx - \omega t)]$$

Answer: $\hbar\omega = \frac{\hbar^2 k^2}{2m} + V(x, t)$

QM-Schrodinger's equation

- Time-independent

If $V(x,t)=V(x)$ only (independent of t) then write Ψ as:

$$\Psi(x, t) = \psi(x)f(t)$$

Separate time-*dependent* Schödinger into two equations:

$$\left\{ \begin{array}{l} f(t) = e^{-i\omega t} \\ \boxed{-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)} \end{array} \right.$$

Time-independent Schrödinger equation (+ boundary conditions).

Energy eigenvalue problem, solve to find energy and $\psi(x)$.

QM-Schrodinger's equation-infinite square well

Example: particle in an infinite square well

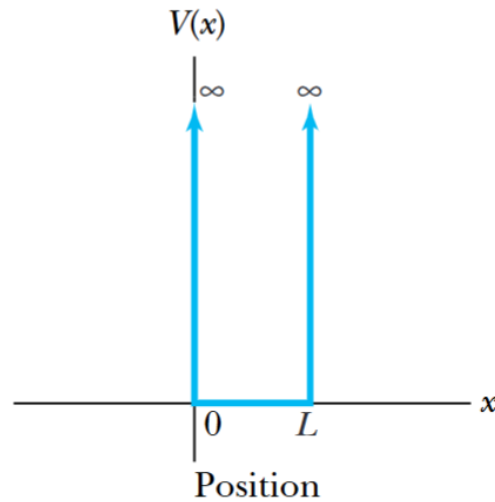


Figure 6.2 Infinite square-well potential. The potential is $V = \infty$ everywhere except the region $0 < x < L$, where $V = 0$.

$$V(x) = \begin{cases} \infty & x \leq 0, x \geq L \\ 0 & 0 < x < L \end{cases}$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (n = 1, 2, 3, \dots)$$

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} \quad (n = 1, 2, 3, \dots)$$

QM-Schrodinger's equation-infinite square well

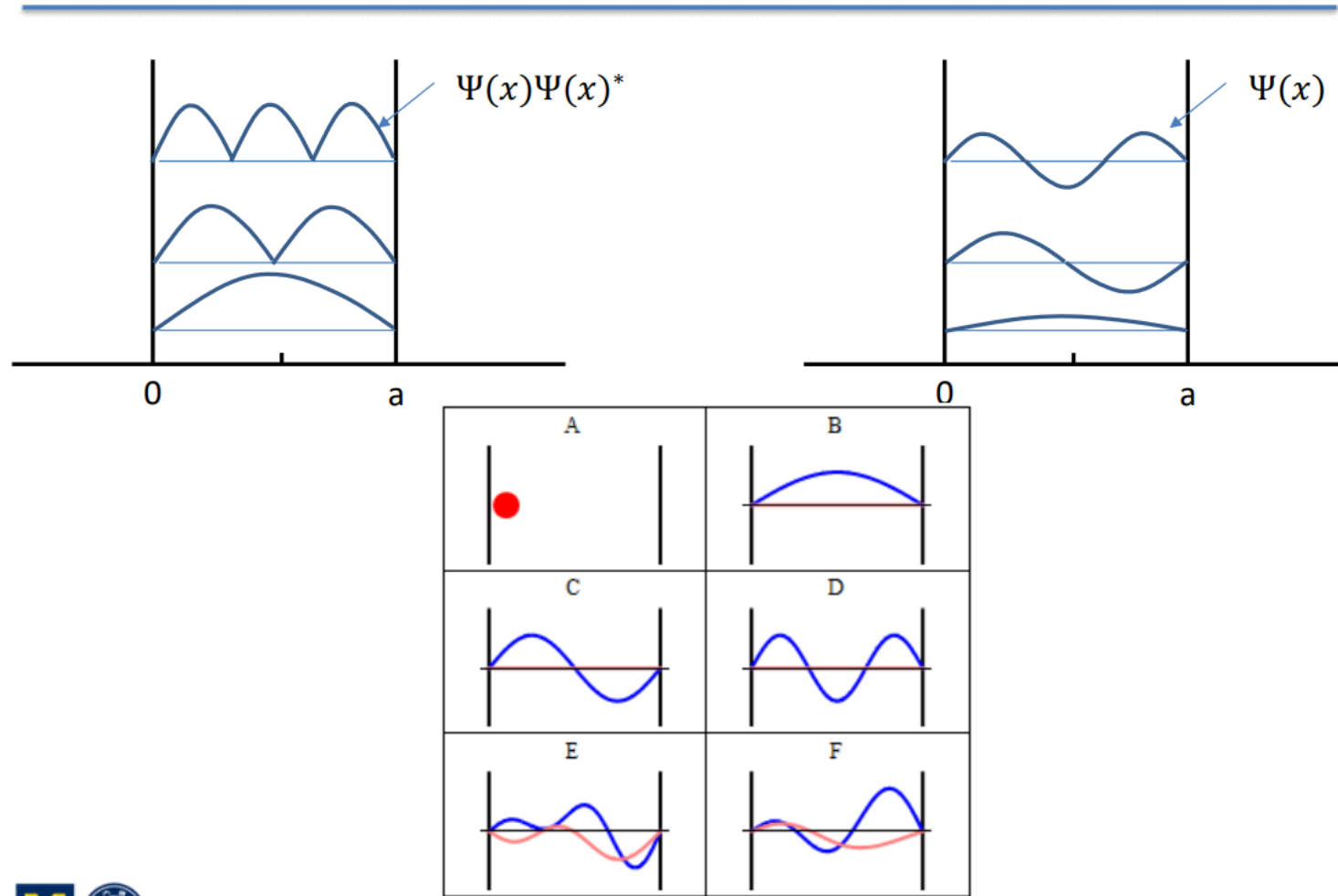
Time-dependent wave function:

$$\Psi_n(x, t) = \psi_n(x)e^{-iE_nt/\hbar} = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \exp\left(-i\frac{E_nt}{\hbar}\right)$$

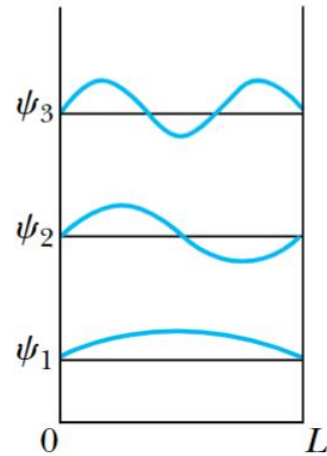
Time dependence adds an oscillatory phase to the wave function.

What is the time dependence of the probability distribution?

QM-Schrodinger's equation-infinite square well



QM-Schrodinger's equation-infinite square well



$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (n = 1, 2, 3, \dots)$$

The set of ψ_n is a **complete** set of wave functions: *any* other wave function that satisfies the same boundary conditions can be written as a **linear combination** of the ψ_n

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

where
$$c_n = \int_{-\infty}^{\infty} \psi_n^*(x) f(x) dx$$

QM-Schrodinger's equation-finite square well

2.5 Electrons in Finite Quantum Well

$$\text{If } E < V_0 \quad k_1 = i \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Boundary Conditions:

$$\Psi(x)|_{x=a,0} \text{ continuous}$$

$$\Psi'(x)|_{x=a,0} \text{ continuous}$$

$$\int_{-\infty}^{\infty} \Psi(x) \Psi^*(x) dx = 1$$

for $x < 0, x > a$

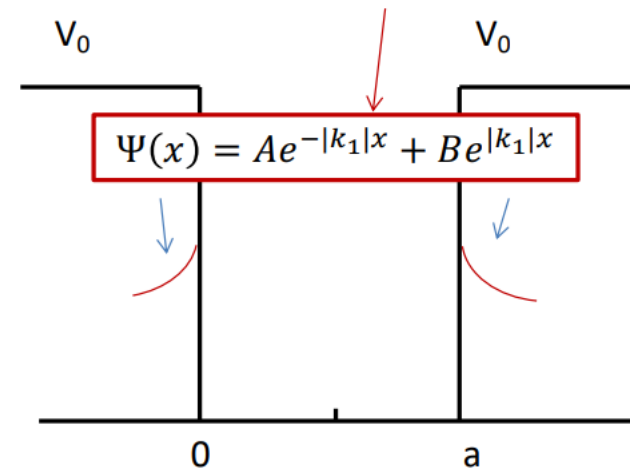
$$\Psi(x) = Ae^{-ik_1x} + Be^{ik_1x}$$

$$k_1 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

for $0 \leq x \leq a$

$$\Psi(x) = Ce^{-ik_2x} + De^{ik_2x}$$

$$k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$



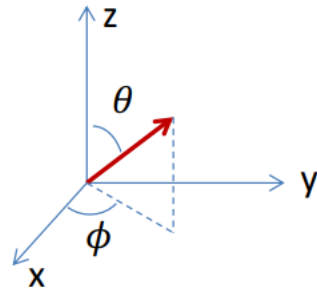
QM-Schrodinger's equation-finite square well

- Note there are two cases, we should compare the electron energy with the potential.

QM-Schrodinger's equation-Hydrogen atom

- The only analytically solved atom

- 3D



$$\Psi_{r,\theta,\phi} = R_n^l(r) Y_l^m(\phi, \theta)$$

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2\mu}{\hbar^2} (E - V) \psi = 0 \quad (7.3)$$

QM-Schrodinger's equation-Hydrogen atom

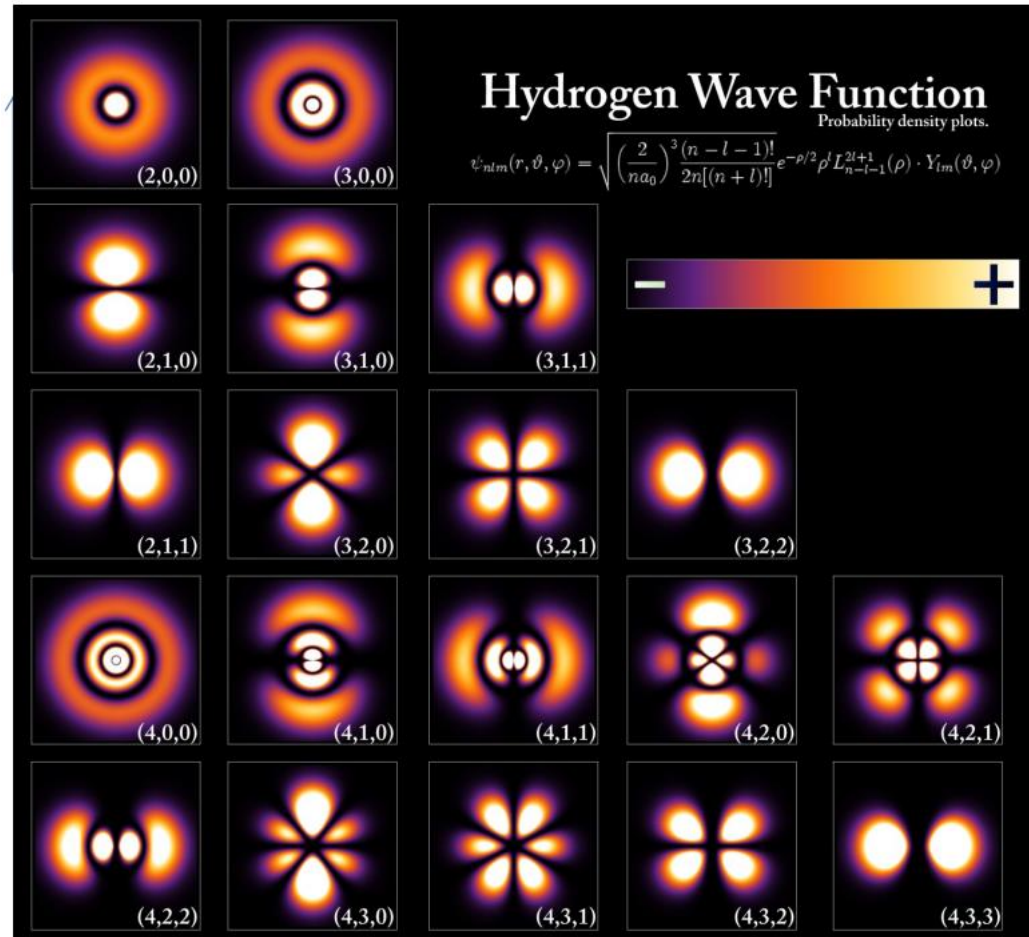
Table 7-1 Spherical harmonics

$\ell = 0$	$m = 0$	$Y_{00} = \sqrt{\frac{1}{4\pi}}$
$\ell = 1$	$m = 1$	$Y_{11} = -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}$
	$m = 0$	$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos \theta$
	$m = -1$	$Y_{1-1} = \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi}$
$\ell = 2$	$m = 2$	$Y_{22} = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{2i\phi}$
	$m = 1$	$Y_{21} = -\sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{i\phi}$
	$m = 0$	$Y_{20} = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$
	$m = -1$	$Y_{2-1} = \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{-i\phi}$
	$m = -2$	$Y_{2-2} = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{-2i\phi}$

Table 7-2 Radial functions for hydrogen

$n = 1$	$\ell = 0$	$R_{10} = \frac{2}{\sqrt{a_0^3}} e^{-r/a_0}$
$n = 2$	$\ell = 0$	$R_{20} = \frac{1}{\sqrt{2a_0^3}} \left(1 - \frac{r}{2a_0} \right) e^{-r/2a_0}$
	$\ell = 1$	$R_{21} = \frac{1}{2\sqrt{6a_0^3}} \frac{r}{a_0} e^{-r/2a_0}$
$n = 3$	$\ell = 0$	$R_{30} = \frac{2}{3\sqrt{3a_0^3}} \left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2} \right) e^{-r/3a_0}$
	$\ell = 1$	$R_{31} = \frac{8}{27\sqrt{6a_0^3}} \frac{r}{a_0} \left(1 - \frac{r}{6a_0} \right) e^{-r/3a_0}$
	$\ell = 2$	$R_{32} = \frac{4}{81\sqrt{30a_0^3}} \frac{r^2}{a_0^2} e^{-r/3a_0}$

QM-Schrodinger's equation-Hydrogen atom



QM-From Hydrogen atom to other atoms

Table 2.1 | Initial portion of the periodic table

Element	Notation	n	l	m	s
Hydrogen	$1s^1$	1	0	0	$+\frac{1}{2}$ or $-\frac{1}{2}$
Helium	$1s^2$	1	0	0	$+\frac{1}{2}$ and $-\frac{1}{2}$
Lithium	$1s^2 2s^1$	2	0	0	$+\frac{1}{2}$ or $-\frac{1}{2}$
Beryllium	$1s^2 2s^2$	2	0	0	$+\frac{1}{2}$ and $-\frac{1}{2}$
Boron	$1s^2 2s^2 2p^1$	2	1	}	$m = 0, -1, +1$ $s = +\frac{1}{2}, -\frac{1}{2}$
Carbon	$1s^2 2s^2 2p^2$	2	1		
Nitrogen	$1s^2 2s^2 2p^3$	2	1		
Oxygen	$1s^2 2s^2 2p^4$	2	1		
Fluorine	$1s^2 2s^2 2p^5$	2	1		
Neon	$1s^2 2s^2 2p^6$	2	1		

QM-Schrodinger's equation-comments

- There are many ways to understand Schrodinger equation, for example, operator view.

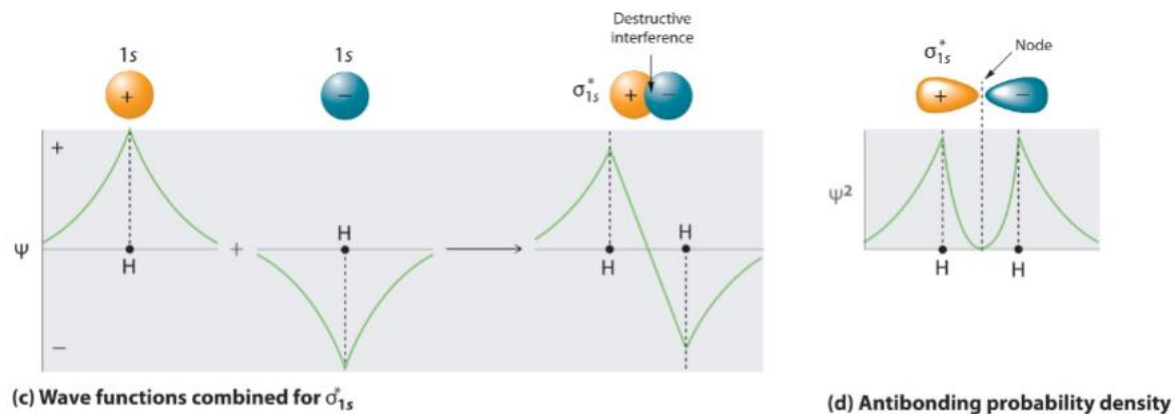
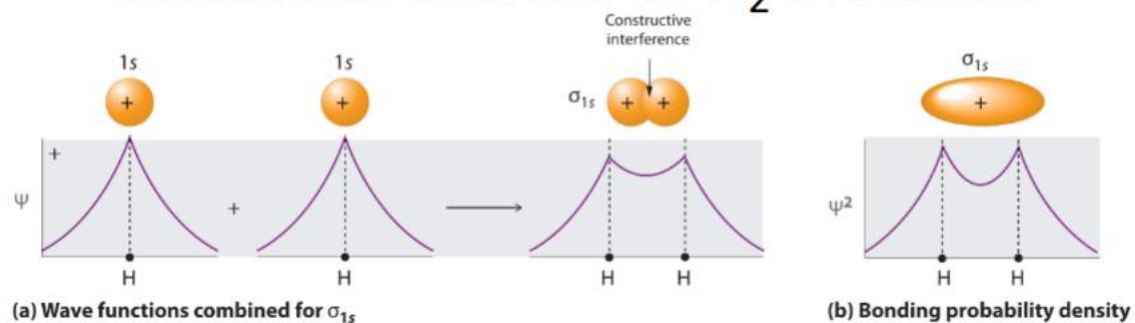
In dealing with classical quantities such as energy E and momentum p , we must relate these quantities with abstract quantum mechanical operators defined in the following way:

Classical variable	Quantum operator
x	x
$f(x)$	$f(x)$
$p(x)$	$\frac{\hbar}{j} \frac{\partial}{\partial x}$
E	$-\frac{\hbar}{j} \frac{\partial}{\partial t}$

- Schrodinger's equation has its limitations, for example, don't include special relativity, don't include electric spin. There's other equation such as Dirac equation.

QM-From one atom to two atoms-Hydrogen example

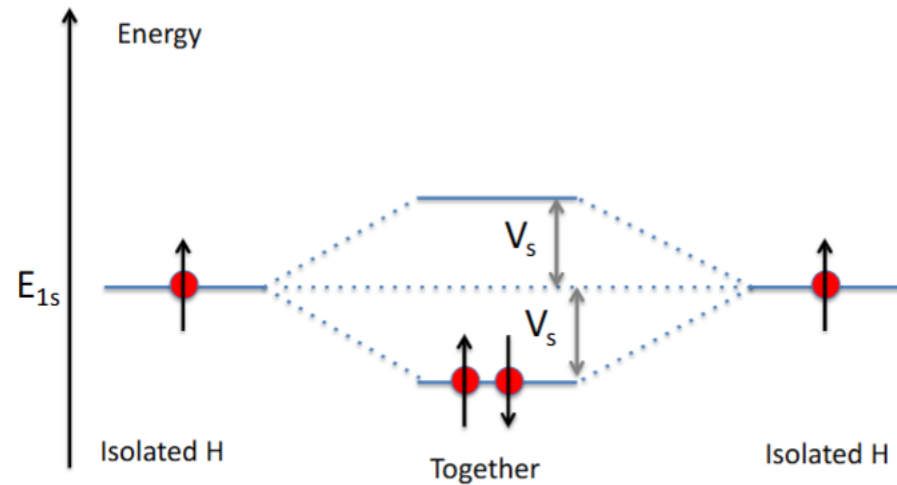
Molecular orbitals of H_2 molecule



[http://chemwiki.ucdavis.edu/Textbook_Maps/General_Chemistry_Textbook_Maps/Map%3A_Chemistry%3A_The_Central_Science_\(Brown_et_al.\)/09._Molecular_Geometry_and_Bonding_Theories/9.7%3A_Molecular_Orbitals](http://chemwiki.ucdavis.edu/Textbook_Maps/General_Chemistry_Textbook_Maps/Map%3A_Chemistry%3A_The_Central_Science_(Brown_et_al.)/09._Molecular_Geometry_and_Bonding_Theories/9.7%3A_Molecular_Orbitals)

QM-From one atom to two atoms-Hydrogen example

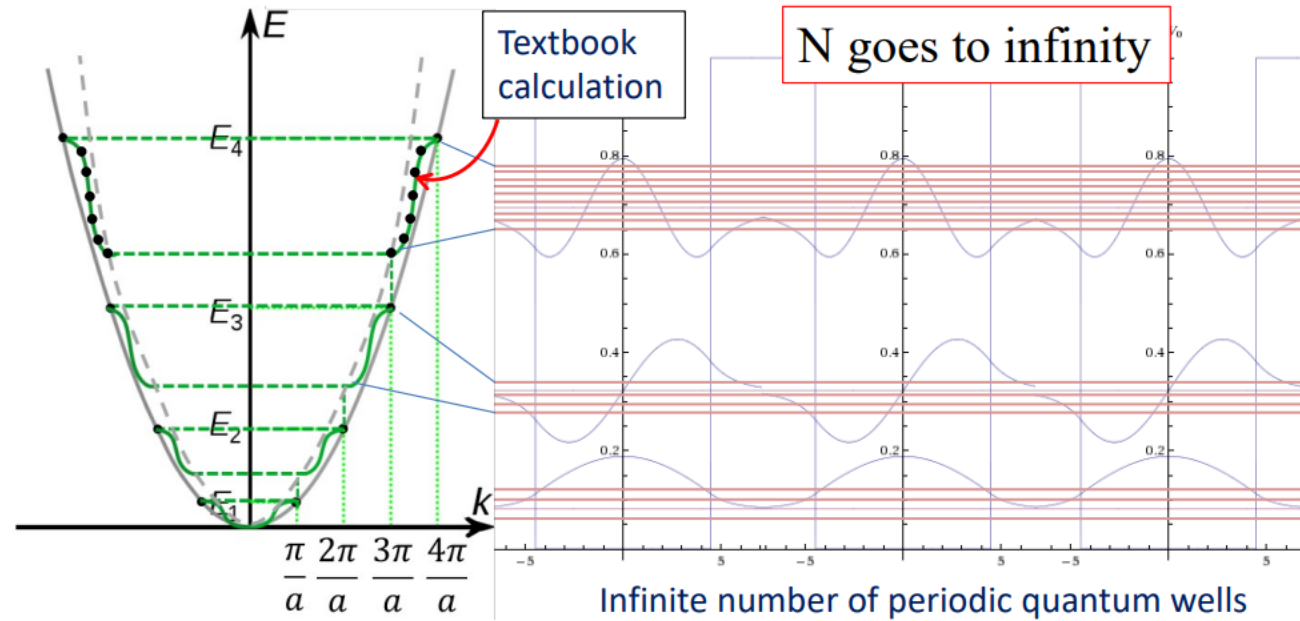
Energies of H_2 molecular orbitals



Question: Does the energy increase or decrease when the two H atoms are brought together? What can you say about bond formation?

QM-From two atoms to a chain of atoms-Band theory

Forming energy bands: analytical

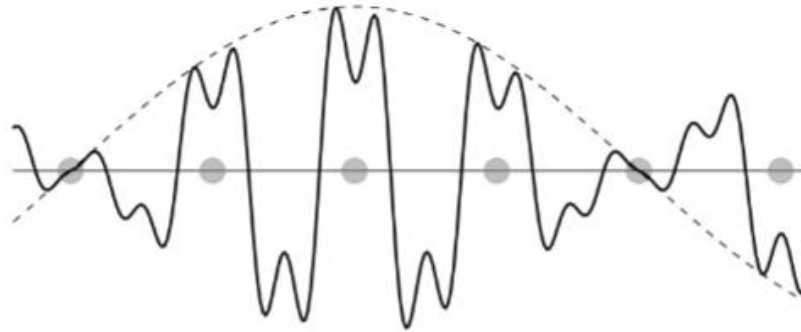


$$\frac{mV_0ba \sin(\alpha a)}{\hbar^2} + \cos(\alpha a) = \cos(ka)$$

On P.67
eq.(3.22)

QM-Band theory-Bloch's theorem

Bloch's theorem



The solution of Schrödinger's equation in a periodic potential is a wave (Bloch wave)

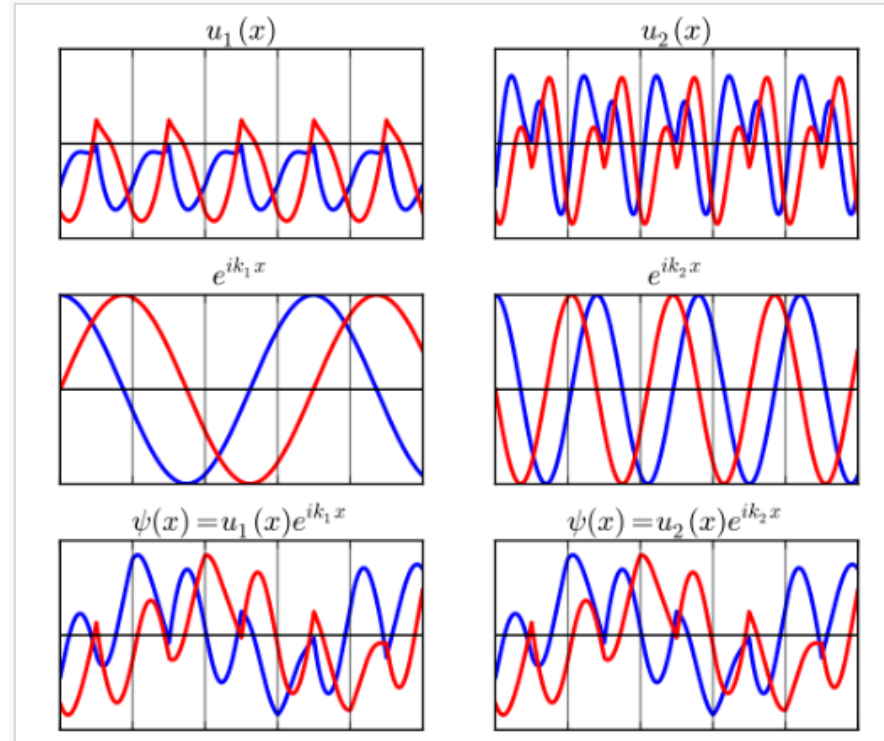
$$\psi(x) = u(x)e^{ikx}$$

$u(x)$ is a periodic function with the same period as the potential (i.e., the period of the crystal).

In contrast: for empty space: $\psi(x) = e^{ikx}$

→ Explains long mean-free paths of electrons in metals.

QM-Band theory-Bloch's theorem-1st Brillouin zone



A Bloch wave function (bottom) can be broken up into the product of a periodic function (top) and a plane-wave (center). The left side and right side represent the same Bloch state broken up in two different ways, involving the wave vector k_1 (left) or k_2 (right). The difference $(k_1 - k_2)$ is a [reciprocal lattice vector](#). In all plots, blue is real part and red is imaginary part.

QM-Band theory-Bloch's theorem-1st Brillouis zone

Band structure in physical and k space for 1D periodic quantum wells

