VE 320 Fall 2021

Introduction to Semiconductor Devices

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Lecture 2

Introduction to quantum mechanics (Chapter 2)

- Why? The revolution of information technology comes from quantum mechanics
- 2/3 of the world GDP comes from quantum mechanics

1927 Solvay Conference

The temple of classical physics

The temple of classical physics

Classical mechanics
- Newton's laws of motion
- Newton’s law of universal gravitation

The temple of classical physics

Statistical mechanics

The temple of classical physics

Electrodynamics
• Maxwell's equations

The dark clouds over classical physics

The dark clouds over classical physics

William Thomson,
1st Baron Kelvin

The dark clouds over classical physics

William Thomson,
1st Baron Kelvin

The dark clouds over classical physics

APPENDIX B.

NINETEENTH CENTURY CLOUDS OVER THE DYNAMICAL THEORY OF HEAT AND LIGHT*.

(Friday evening Lecture, Royal Institution, April 27, 1900.)

[IN the present article the substance of the lecture is reproduced—with large additions, in which work commenced at the beginning of last year and continued after the lecture, during thirteen months up to the present time, is described—with results confirming the conclusions and largely extending the illustrations which were given in the lecture. I desire to take this opportunity of expressing my obligations to Mr William Anderson, my secretary and assistant, for the mathematical tact and skill, the accuracy of geometrical drawing, and the unfailingly faithful perseverance in the long-continued and varied series of drawings and algebraic and arithmetical calculations, explained in the following pages. The whole of this work, involving the determination of results due to more than five thousand individual impacts, has been performed by Mr Anderson.—K., Feb. 2, 1901.]

§ 1. The beauty and clearness of the dynamical theory, which asserts heat and light to be modes of motion, is at present obscured by two clouds. I. The first came into existence with the undulatory theory of light, and was dealt with by Fresnel and Dr Thomas Young; it involved the question, How could the earth move through an elastic solid, such as essentially is the luminiferous ether? II. The second is the Maxwell-Boltzmann doctrine regarding the partition of energy.

§ 2. CLOUD I.—RELATIVE MOTION OF ETHER AND PONDERABLE BODIES; such as movable bodies at the earth's surface, stones, metals, liquids, gases; the atmosphere surrounding the earth; the earth itself as a whole; meteorites, the moon, the sun,

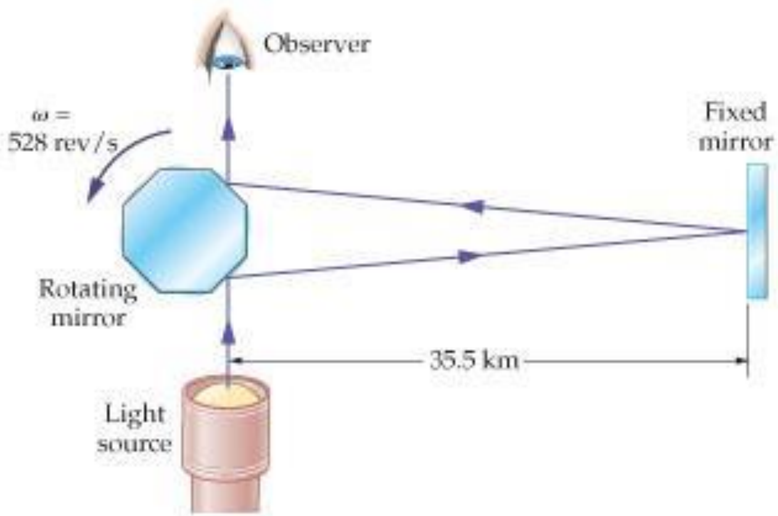
* *Journal of the Royal Institution.* Also *Phil. Mag.* July, 1901.

- Light is particle or wave?
- Blackbody radiation
  - When black body radiates, the emitted energy must be carried by DISCRETE packet of energy
  - Planck named it “quantum”

Introduction to quantum mechanics

- Historic development of quantum mechanics

① Speed of light in 1862 $v = 2.98 \times 10^8 m/s$



Rotation mirror

Leon Foucault

Introduction to quantum mechanics

- Historic development of quantum mechanics

② Maxwell Equations in the year 1865

$$\begin{cases} \nabla \cdot E = 4\pi\rho \\ \nabla \times E = -\dfrac{1}{\sqrt{\mu\varepsilon}}\dfrac{\partial B}{\partial t} \\ \nabla \cdot B = 0 \\ \nabla \times B = \dfrac{4\pi}{c}J + \dfrac{1}{\sqrt{\mu\varepsilon}}\dfrac{\partial E}{\partial t} \end{cases}$$

James Maxwell

Static differential equation describing the electromagnetic wave

$$\frac{\partial^2 E_x}{\partial x^2} = -\omega^2 \mu\varepsilon E_x \qquad E_x = E_{x0} e^{-i\omega\sqrt{\mu\varepsilon}x}$$

Light is an electromagnetic wave!

$$v = \frac{1}{\sqrt{\mu\varepsilon}} = 2.99 \times 10^8 m/s$$

Introduction to quantum mechanics

③ Light wave-particle duality in 1905

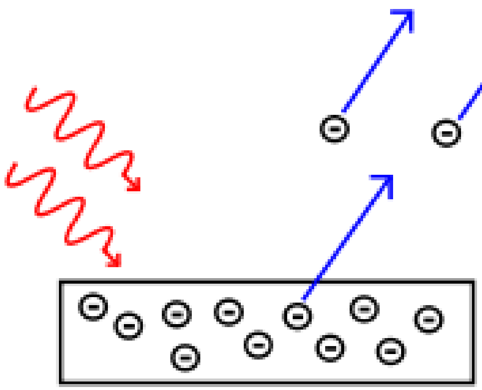
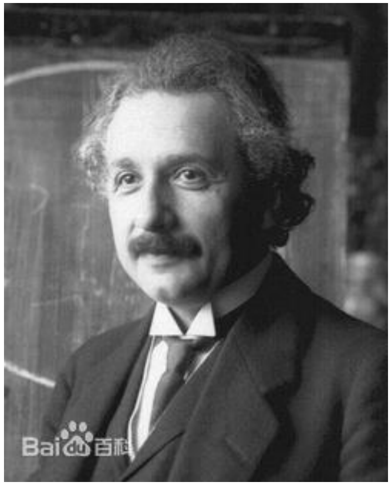


Photo-electric experiment

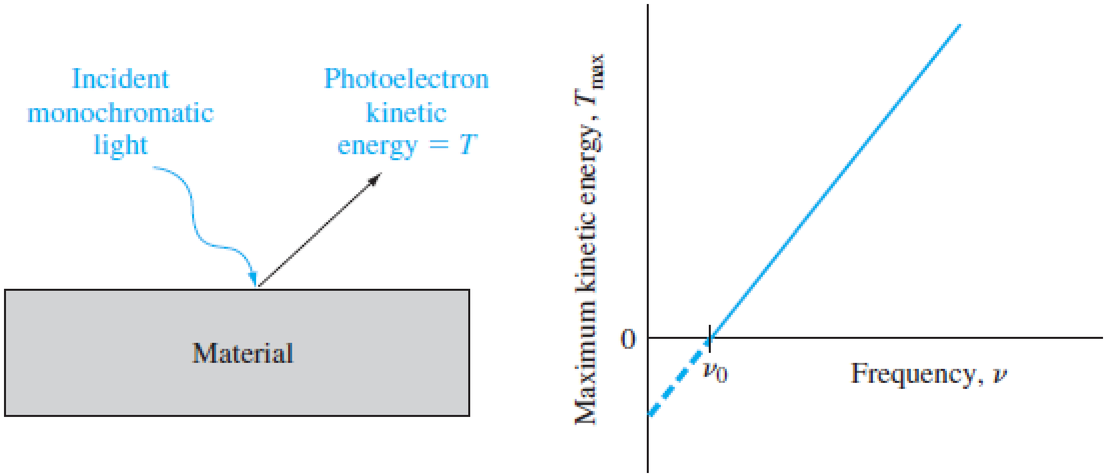


Albert Einstein
Nobel Prize 1921

- Light frequency higher than a certain frequency → election ejection
- Not a function of light intensity
- Light wave is a particle: $h\nu = T_{max} + \Phi$

Introduction to quantum mechanics

③ Light wave-particle duality in 1905



- Plot of the maximum kinetic energy of ejected electrons vs. frequency of the incoming light
- Only the number of electrons is proportional to the intensity of light
- The energy of the photoelectron only depends on the wavelength
- Some wavelength doesn't generate any photoelectron

Introduction to quantum mechanics

③ Light wave-particle duality in 1905

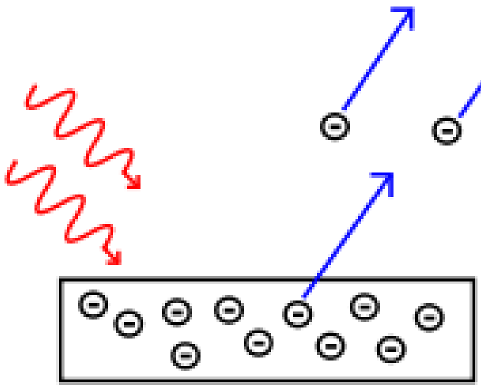
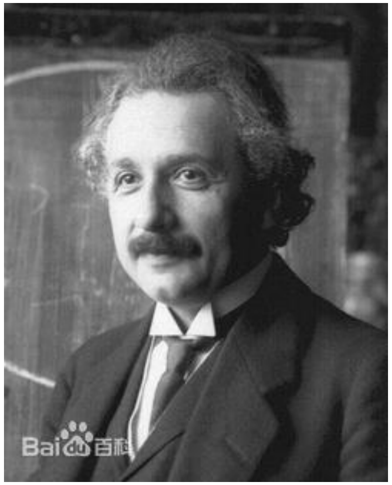


Photo-electric experiment



Albert Einstein
Nobel Prize 1921

$$E = h\text{v} = \hbar\omega \qquad\qquad E = mc^2$$

$$\text{p} = mc = \frac{E}{c} = \frac{h\text{v}}{c} = \frac{h}{\lambda} = \hbar k$$

Light is a particle!

$$k = \frac{2\pi}{\lambda}$$

Introduction to quantum mechanics

④ Matter wave hypothesis in 1924

Louis Victor de Broglie
Nobel Prize 1929

$$E = \frac{1}{2}mv^2 \qquad E = h\mathrm{v} = \hbar\omega$$

$$\mathrm{p} = mv \qquad \mathrm{p} = \frac{h}{\lambda} = \hbar k$$

Matter particle — Wave- particle

Quantum mechanics – introduction

- Quantum mechanics: A method to explain the behavior of fundamental (small) particles (e.g., electrons, photons) because these particles don't follow classical mechanics.
- Classic Experiments leading to Quantum Mechanics:

– Planck's observations of emitting bodies: (they emit light)

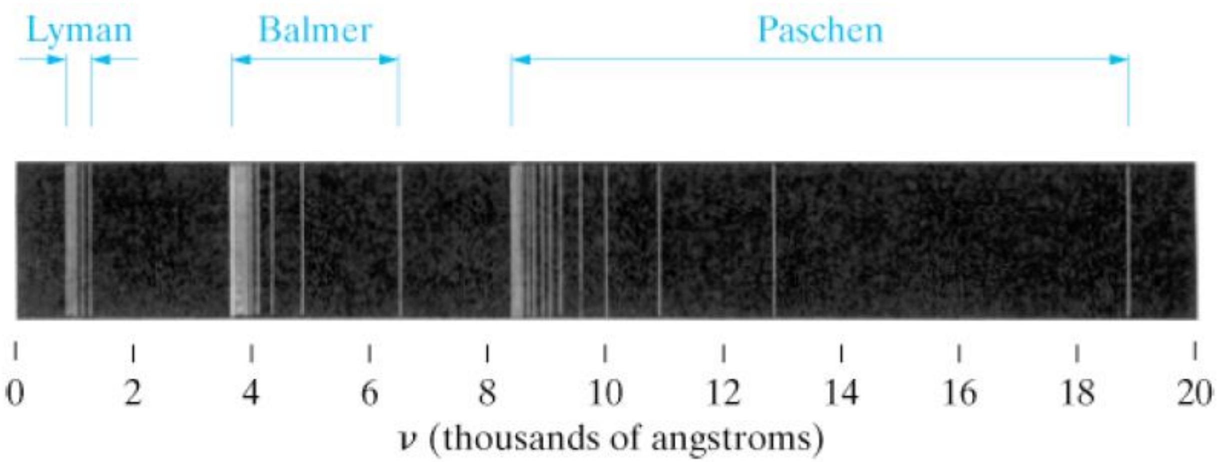
– Photoelectric effect: (light interacts with electrons)

– Atomic emission spectra: (light emission is quantized)

– Bohr model of hydrogen atom: (e- in discrete orbits with distinct energies, transitions related to photons).

Atomic emission spectra

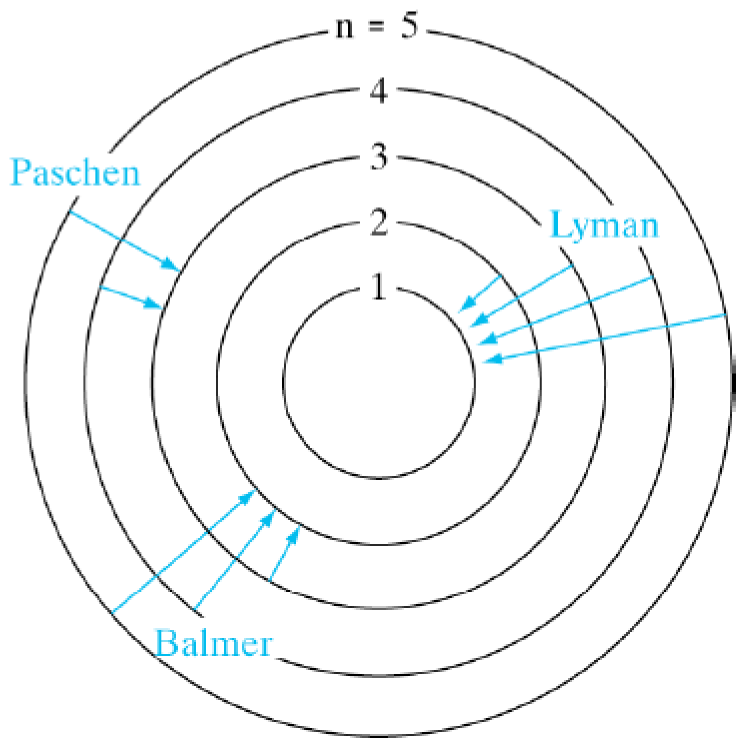
- When an electric discharge is generated in a gas, emission of light at characteristic, discrete wavelengths occurs.
- Hydrogen, the simplest atom, is the easiest to study.
- Emission from hydrogen falls into 3 distinct groups.



- Some important lines in the emission spectrum of hydrogen.
- The emission is quantized.

The Bohr Model

- Objective – To describe the electronic structure of the hydrogen atom consistent with experimental observations.
- Key feature: Electrons exist in stable orbits about a nucleus.
- Postulates:
  - Electron orbits are circular. Multiple orbits possible.
  - Orbits represent energy levels.
  - Electrons can transit from one orbit to another.
  - Transitions require a change in energy that is equivalent to the energy differences of the orbits.
  - Changes in electron energy occur either by the absorption of light (photoelectric effect) or emission of light (atomic spectra).



Electron orbits and transitions in the Bohr model of the hydrogen atom.

- The Bohr model of the (isolated) Si atom (N. Bohr, 1913):

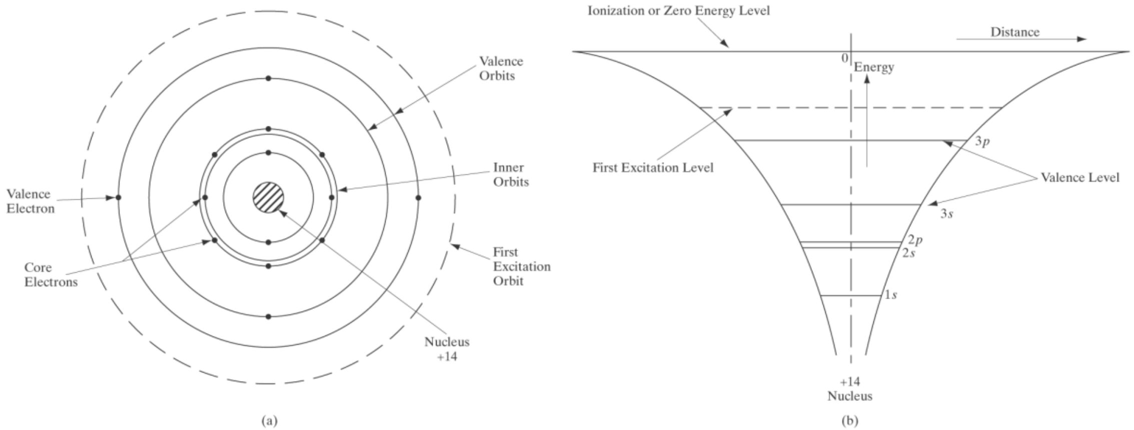


Figure 2.8

Electronic structure and energy levels in a Si atom: (a) The orbital model of a Si atom showing the 10 core electrons (**n** = 1 and 2), and the 4 valence electrons (**n** = 3); (b) energy levels in the coulombic potential of the nucleus are also shown schematically.

- Note: inner shell electrons *screen* outer shell electrons from the positive charge of the nucleus (outer less tightly bound)

- Bohr model: $$E_H = -\frac{mq^4}{2\left(4\pi\varepsilon\hbar\mathbf{n}\right)^2} = -\frac{13.6}{\mathbf{n}^2}\,\mathrm{eV}$$

- Uncertainty principle
- The first statement of the uncertainty principle is that it is impossible to simultaneously describe with absolute accuracy the position and momentum of a particle

$$\Delta p \, \Delta x \geq \hbar$$

where $\hbar$ is defined as $\hbar = h/2\pi = 1.054 \times 10^{-34}$ J-s and is called a modified Planck's constant

- The second statement of the uncertainty principle is that it is impossible to simultaneously describe with absolute accuracy the energy of a particle and the instant of time the particle has this energy.

$$\Delta E \, \Delta t \geq \hbar$$

- We cannot determine the exact position of an electron. We will, instead, determine the probability of finding an electron at a particular position.

Schrodinger wave equation (1926)

- Three-dimensional

$$j\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

- One-dimensional (time-dependent)

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

wave function Ψ(x,t) *can be complex!*

- Separation of variables

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

Schrodinger wave equation (1926)

- Equation becomes:

$$\frac{-\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = j\hbar\cdot\frac{1}{\phi(t)}\cdot\frac{\partial\phi(t)}{\partial t}$$

- Equation 1: with time

$$\eta = j\hbar\cdot\frac{1}{\phi(t)}\cdot\frac{\partial\phi(t)}{\partial t}$$

- Solution: $\phi(t) = e^{-j(\eta/\hbar)t}$

$$\phi(t) = e^{-j(E/\hbar)t} = e^{-j\omega t}$$

$\omega = E/\hbar$ $\quad$ $\eta=E$

Schrodinger wave equation (1926)

- Time-independent Schrodinger's wave equation:

$$\frac{-\hbar^2}{2m} \cdot \frac{1}{\psi(x)} \cdot \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = E$$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

Physical meaning of wave function

$$\Psi(x, t) = \psi(x)\,\phi(t) = \psi(x)e^{-j(E/\hbar)t} = \psi(x)e^{-j\omega t}$$

Max Born: $|\Psi(x, t)|^2 = \Psi(x, t) \cdot \Psi^*(x, t)$

is the probability of finding the particle between x and x+dx at a given time, or that $|\Psi(x, t)|^2$ is a probability density function.

$$\Psi^*(x, t) = \psi^*(x) \cdot e^{+j(E/\hbar)t}$$

$$|\Psi(x, t)|^2 = \psi(x)\psi^*(x) = |\psi(\chi)|^2$$

Probability density function is independent of time

Physical meaning of wave function

We have to find the particle somewhere.

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

Boundary conditions:
If the total energy *E* and the potential *V* (*x*) are finite everywhere
Condition 1. $\psi(x)$ must be finite, single-valued, and continuous.
Condition 2. $\partial\psi(x)/\partial x$ must be finite, single-valued, and continuous.

Introduction to quantum mechanics

- 2nd order differential equation and waves

$$\frac{\partial^2 y}{\partial x^2} = k^2 y$$

General solution: $y = Ae^{bx}$

Plug into the equation: $b^2 A e^{bx} = k^2 A e^{bx}$

$$\Rightarrow b = \pm k$$

$$\Rightarrow y = A_1 e^{kx} + A_2 e^{-kx}$$

Introduction to quantum mechanics

- 2^{nd} order differential equation and waves

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$$\Rightarrow y = A_1 e^{kx} + A_2 e^{-kx}$$

$$\frac{\partial^2 y}{\partial x^2} = -k^2 y$$

General solution: $y = Ae^{bx}$

Plug into the equation: $b^2 Ae^{bx} = -k^2 Ae^{bx}$

$$\Rightarrow b = \pm kj$$

$$\Rightarrow y = A_1 e^{jkx} + A_2 e^{-jkx}$$

Introduction to quantum mechanics

- 2^{nd} order differential equation and waves

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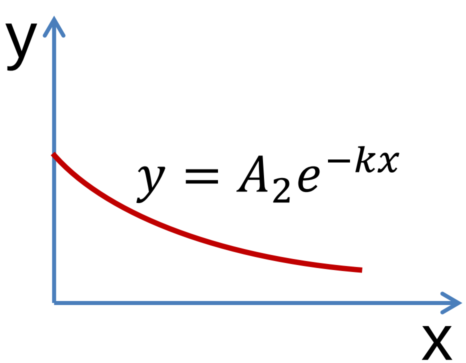
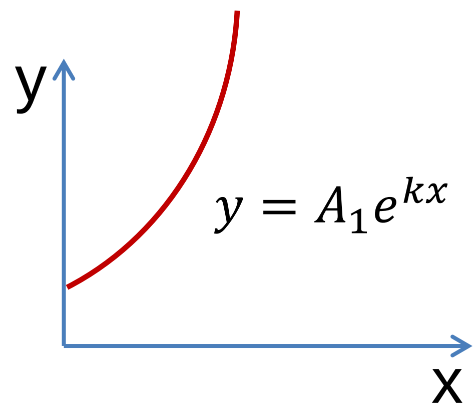
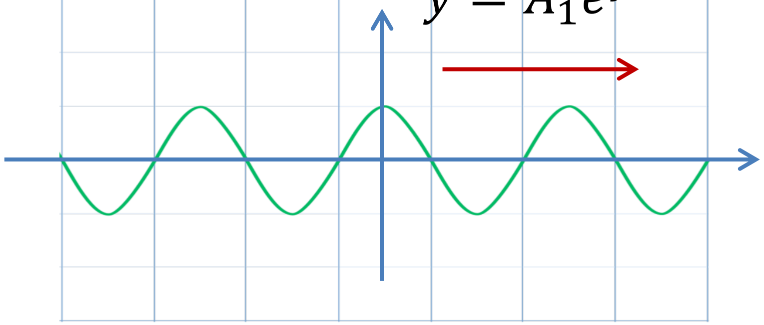
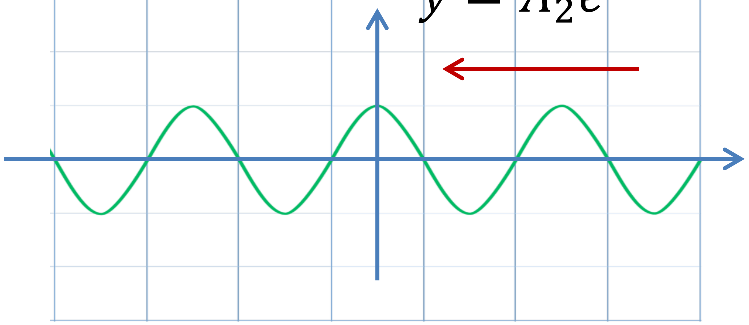




Introduction to quantum mechanics

- 2^{nd} order differential equation and waves





$$\frac{\partial^2 y}{\partial x^2} = -k^2 y$$

General solution: $y = Ae^{bx}$

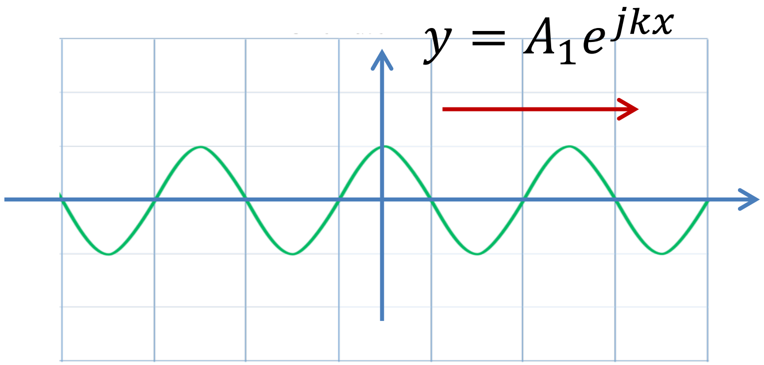
Plug into the equation: $b^2 A e^{bx} = -k^2 A e^{bx}$

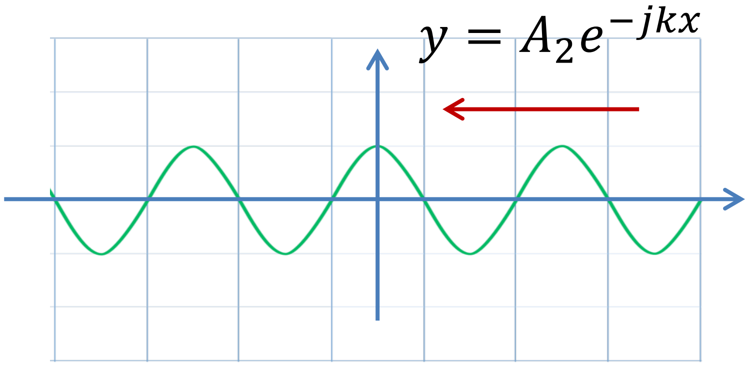
$$\Rightarrow b = \pm kj$$

$$\Rightarrow y = A_1 e^{jkx} + A_2 e^{-jkx}$$

Introduction to quantum mechanics

- 2^{nd} order differential equation and waves





1. Give a wave propagating along x with a wavelength λ_0, please write the static 2^{nd} order differential equation that governs the behavior of this wave.

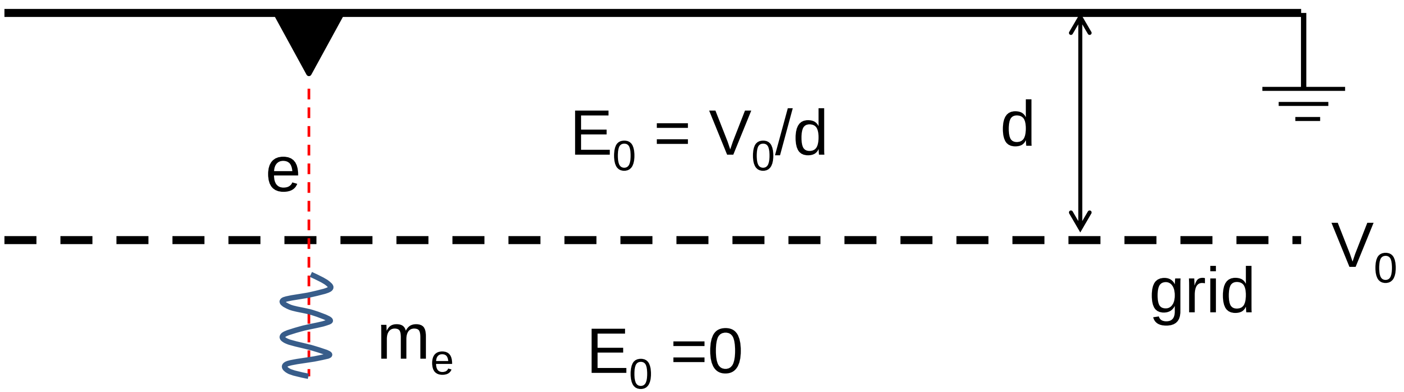
Introduction to quantum mechanics

- Maxwell Equation in the year 1865
- Light wave-particle duality in 1905
- Matter wave hypothesis in 1924

$$\frac{\partial^2 y}{\partial x^2} = -k^2 y$$

$$E = \frac{1}{2}mv^2 \qquad E = h\text{v} = \hbar\omega$$

$$\text{p} = mv \qquad \text{p} = \frac{h}{\lambda} = \hbar k$$



Can you find a differential equation that governs the wave behavior of electrons?

Introduction to quantum mechanics

$$E = qV_0 = \frac{1}{2}mv^2$$

$$\mathrm{p} = mv$$

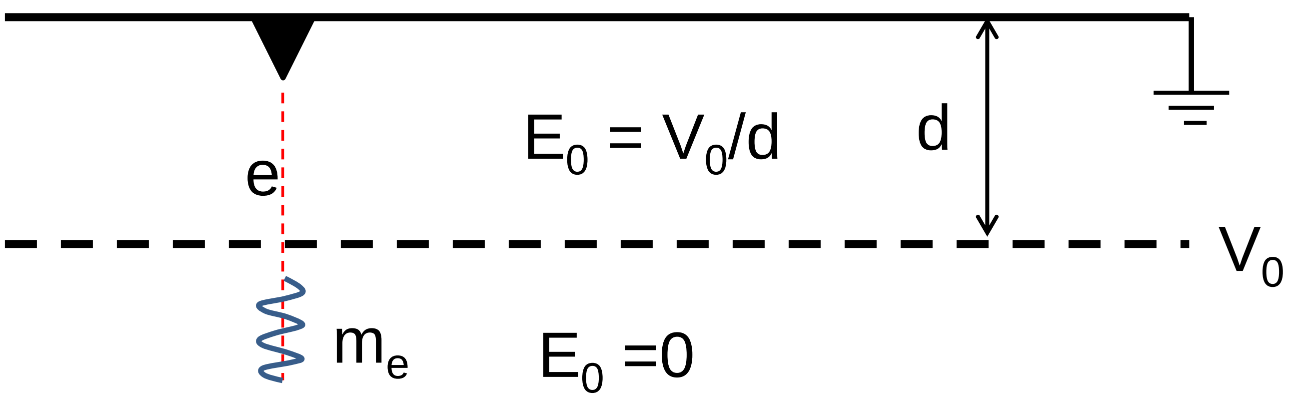
$$E = h\mathrm{v} = \hbar\omega$$

$$\mathrm{p} = \frac{h}{\lambda} = \hbar k$$

$$v = \sqrt{\frac{2qV_0}{m}}$$

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi = -\frac{2mqV_0}{\hbar^2}\psi$$

$$k = \frac{m}{\hbar}v = \sqrt{\frac{2mqV_0}{\hbar^2}}$$



Can you find a differential equation that governs the wave behavior of electrons?

Introduction to quantum mechanics

$$E = qV_0 = \frac{1}{2}mv^2 \qquad E = h\text{v} = \hbar\omega \qquad v = \sqrt{\frac{2qV_0}{m}}$$

$$\text{p} = mv \qquad \text{p} = \frac{h}{\lambda} = \hbar k$$

$$k = \frac{m}{\hbar}v = \sqrt{\frac{2mqV_0}{\hbar^2}}$$

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi = -\frac{2mqV_0}{\hbar^2}\psi$$

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi = -\frac{2mE}{\hbar^2}\psi$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi}$$

Time-independent Schrodinger Equation !

Introduction to quantum mechanics

$$E = qV_0 = \frac{1}{2}mv^2 \qquad E = h\nu = \hbar\omega$$

$$\mathrm{p} = mv \qquad \mathrm{p} = \frac{h}{\lambda} = \hbar k \qquad v = \sqrt{\frac{2qV_0}{m}}$$

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi = -\frac{2mqV_0}{\hbar^2}\psi \qquad k = \frac{m}{\hbar}v = \sqrt{\frac{2mqV_0}{\hbar^2}}$$

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi = -\frac{2mE}{\hbar^2}\psi$$

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

Schrodinger Equation !

Electrons in free space

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi}$$

$$V(x) = 0$$

Solution:

$$\psi(x) = A\exp\left[\frac{jx\sqrt{2mE}}{\hbar}\right] + B\exp\left[\frac{-jx\sqrt{2mE}}{\hbar}\right]$$

Or:

$$\psi(x) = A\exp(jkx) + B\exp(-jkx)$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{p}{\hbar}$$ is the wave number

$$\lambda = \frac{h}{p} = \frac{2\pi\hbar}{p} \qquad \lambda = \frac{2\pi}{k}$$ Wavelength!

Electrons in Infinite Quantum Well

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

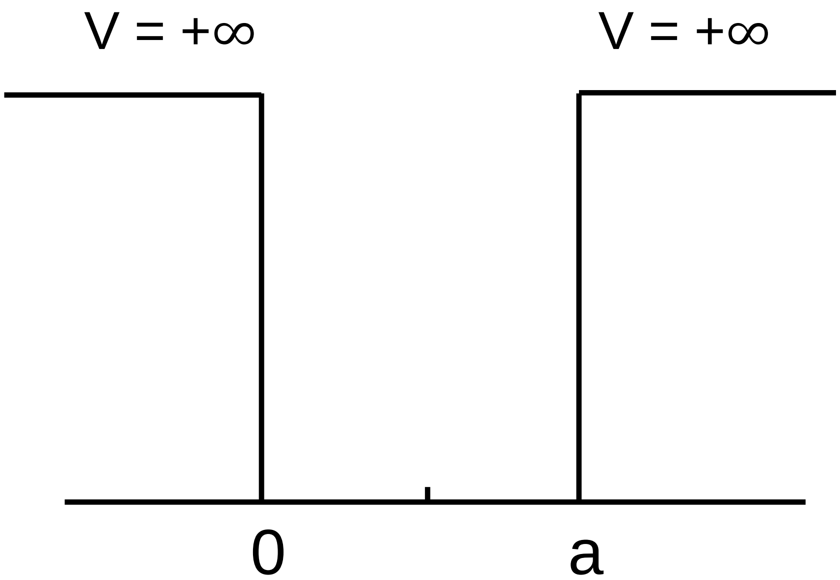
Conditions:

$$for\ x<0, x>a$$

$$V(x)=+\infty;$$

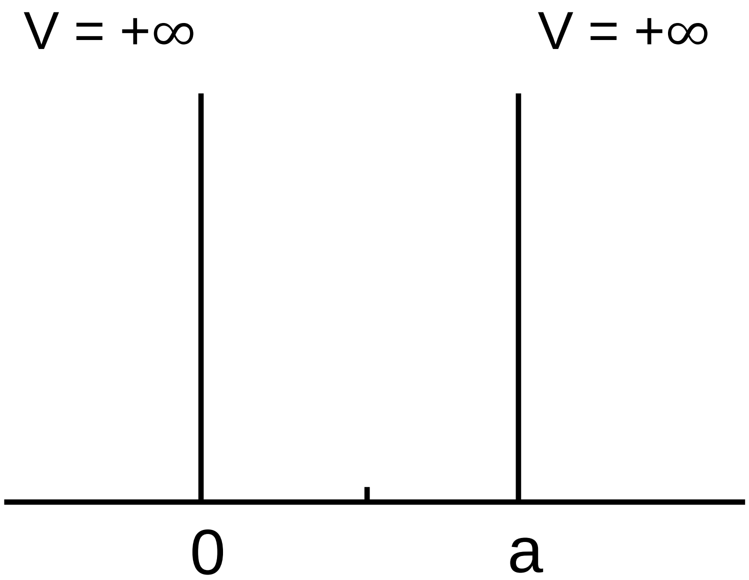
$$for\ 0\leq x\leq a$$

$$V(x)=0$$



Electrons in Infinite Quantum Well

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



Conditions:

$$for\; x<0, x>a$$

$$V(x)=+\infty; \Rightarrow \psi(x)=0$$

$$for\; 0\le x\le a$$

$$V(x)=0$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}=E\psi} \Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2}=-\frac{2mE}{\hbar^2}\psi} \Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2}=-k^2\psi}$$

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

Electrons in Infinite Quantum Well

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi} \Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi} \Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2} = -k^2\psi}$$

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

The general solution

$$\boxed{\psi(x) = Ae^{-jkx} + Be^{jkx}}$$

Boundary conditions:

$$\begin{cases} \psi(x)|_{x=a,0} = 0 \\ \int_0^a \psi(x)\psi^*(x)dx = 1 \end{cases}$$

Electrons in Infinite Quantum Well

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}=E\psi} \Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2}=-\frac{2mE}{\hbar^2}\psi} \Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2}=-k^2\psi}$$

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

The general solution

$$\boxed{\psi(x)=Ae^{-jkx}+Be^{jkx}}$$

Boundary conditions:

$$\begin{cases}\psi(x)|_{x=a,0}=0 \\ \int_0^a \psi(x)\psi^*(x)dx=1\end{cases} \Rightarrow \begin{array}{l}\boxed{\psi(x)=Ae^{-jk0}+Be^{jk0}=0\Rightarrow A=-B} \\ \boxed{\psi(x)=Ae^{-jka}+Be^{jka}=0\Rightarrow \sin(ka)=0}\end{array}$$

$$ka=n\pi \quad where\, n=0,\pm1,\pm2,\ldots$$

Negative *n*: redundant for probability density function, ignored

$$n=0,1,2,\ldots$$

Electrons in Infinite Quantum Well

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi} \Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi} \Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2} = -k^2\psi}$$

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

The general solution

$$\boxed{\psi(x) = (B - A)jsin(kx) = A_2\sin(kx)}$$

From book

Boundary conditions:

$$\begin{cases} \psi(x)|_{x=a,0} = 0 \\ \int_0^a \psi(x)\psi^*(x)dx = 1 \end{cases} \Rightarrow$$

$$k = \frac{n\pi}{a} \quad n = 0, 1, 2, \ldots$$

$$\mathrm{E} = \frac{k^2\hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Energy is quantized!

Electrons in Infinite Quantum Well

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi} \Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi} \Rightarrow \boxed{\frac{\partial^2\psi}{\partial x^2} = -k^2\psi}$$

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

The general solution

$$\boxed{\psi(x) = (B-A)j\sin(kx) = A_2\sin(kx)}$$

Boundary conditions:

$$\begin{cases} \psi(x)|_{x=a,0} = 0 \\ \int_0^a \psi(x)\psi^*(x)dx = 1 \end{cases} \Rightarrow \int_0^a A_2^2 \sin^2 kx\, dx = 1$$

$A_2^2=2/a$

$$\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \qquad \text{where } n = 1, 2, 3, \ldots$$

Electrons in Infinite Quantum Well

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

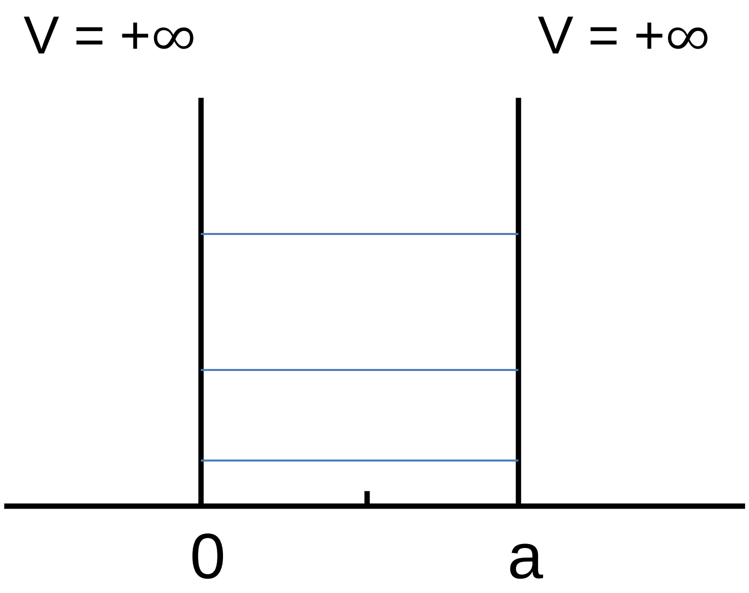
Conditions:

$$for\; x<0, x>a$$

$$V(x)=+\infty;\psi(x)=0$$

$$for\; 0\le x\le a$$

$$V(x)=0$$

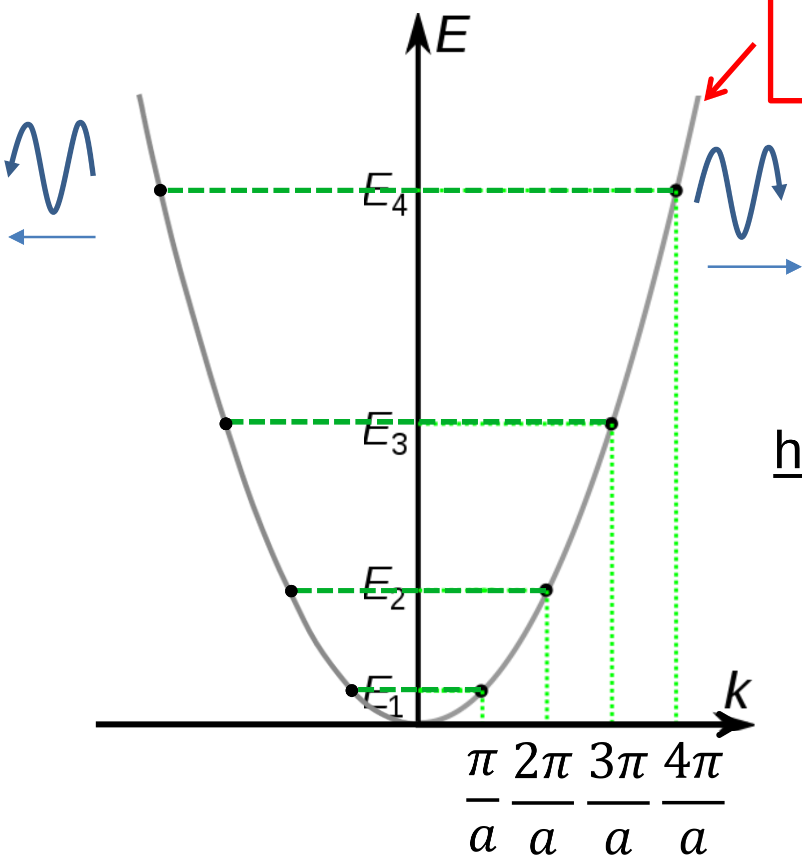


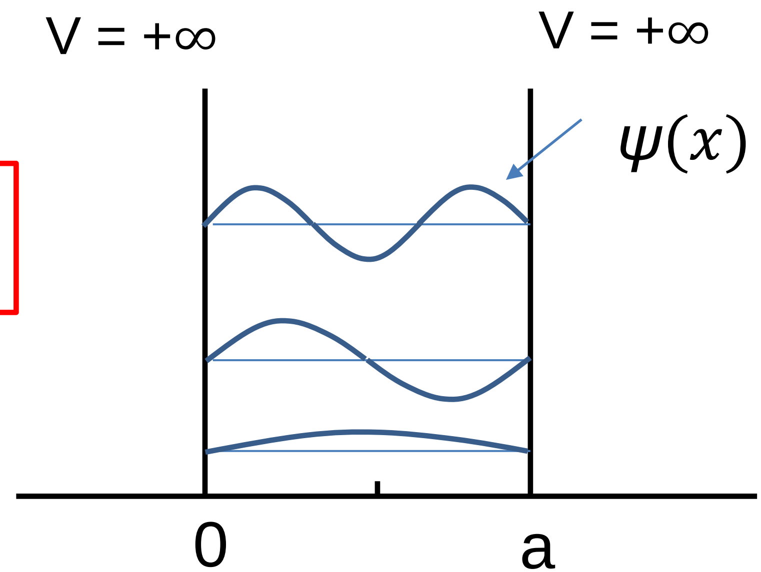
$$\mathrm{E}=\frac{k^2\hbar^2}{2m}=\frac{n^2\pi^2\hbar^2}{2ma^2}$$

Electrons in Infinite Quantum Well

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

$$\boxed{\mathrm{E}=\frac{k^2\hbar^2}{2m}}$$



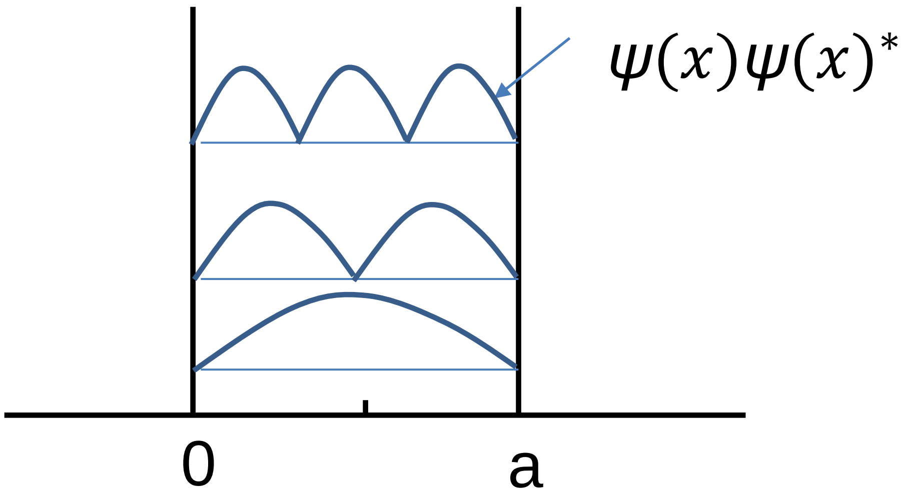


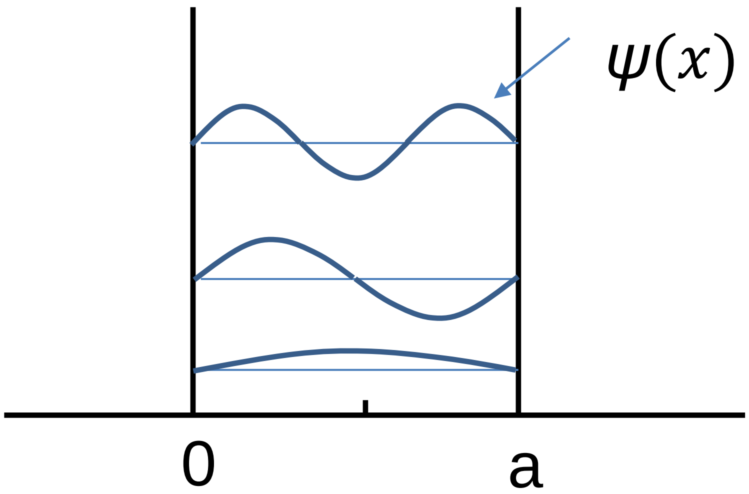
http://en.wikipedia.org/wiki/Particle_in_a_box

$$\mathrm{E}=\frac{k^2\hbar^2}{2m}=\frac{n^2\pi^2\hbar^2}{2ma^2}$$

$$k=\frac{n\pi}{a}\qquad n=0,1,2,\ldots$$

Electrons in Infinite Quantum Well





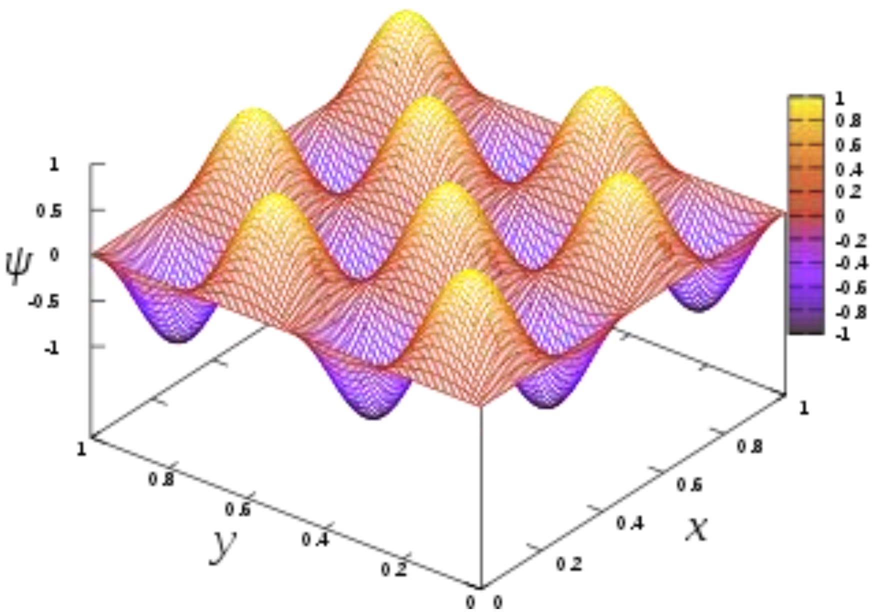
http://en.wikipedia.org/wiki/Particle_in_a_box

$$\mathrm{E} = \frac{k^2\hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

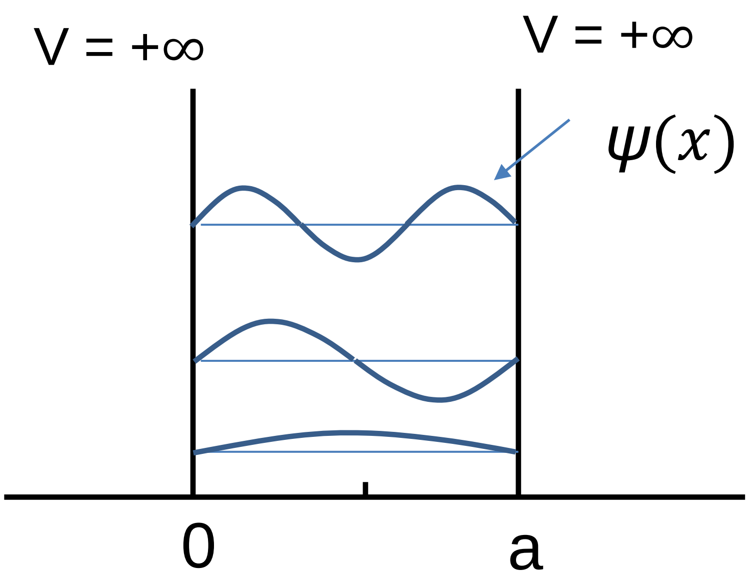
$$k = \frac{n\pi}{a} \quad n = 0, 1, 2, \ldots$$

Electrons in Infinite Quantum Well

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



2-dimentional
Quantum well



$$\mathrm{E}=\frac{k^2\hbar^2}{2m}=\frac{n^2\pi^2\hbar^2}{2ma^2}$$

Electrons in Finite Quantum Well

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

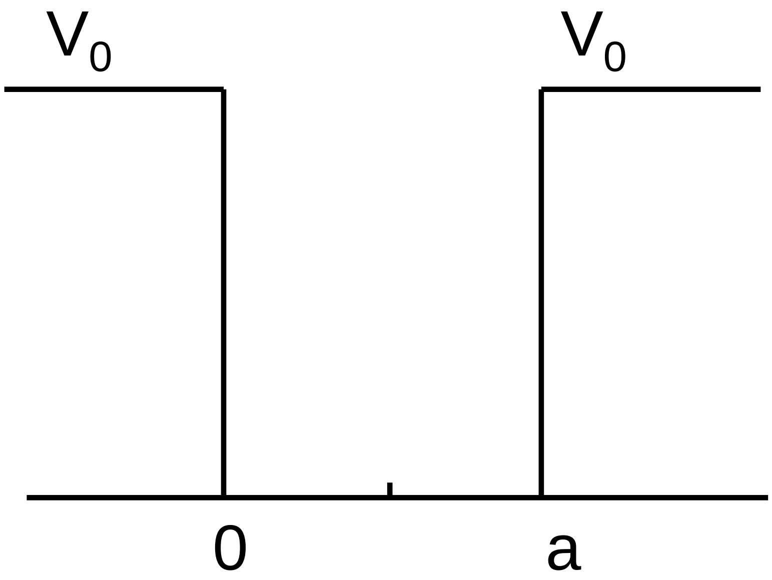
Conditions:

$$for\ x < 0, x > a$$

$$V(x) = V_0;$$

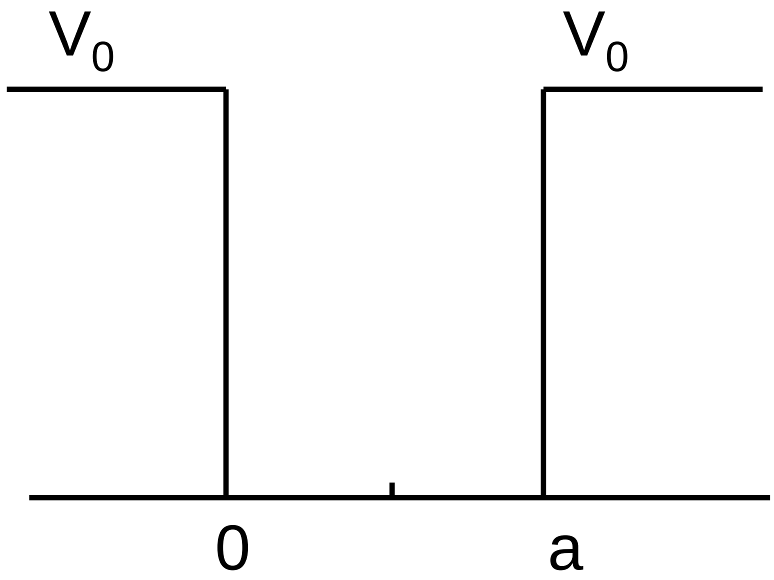
$$for\ 0 \le x \le a$$

$$V(x) = 0$$



Electrons in Finite Quantum Well

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



Conditions:

$$for\ x<0\ x>a$$

$$V(x)=V_0;$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}=(E-V_0)\psi}$$

$$\boxed{\psi(x)=Ae^{-jk_1x}+Be^{jk_1x}}$$

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

$$for\ 0\le x\le a$$

$$V(x)=0$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}=E\psi}$$

$$\boxed{\psi(x)=Ce^{-jk_2x}+De^{jk_2x}}$$

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

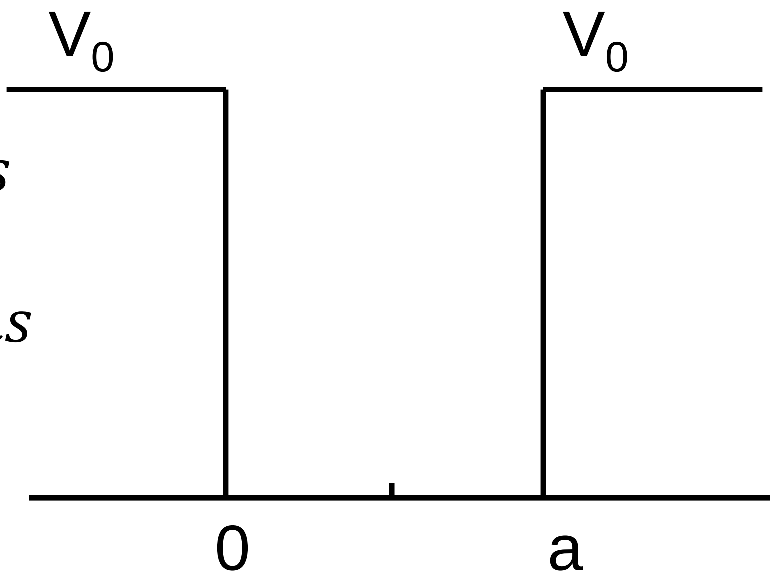
Electrons in Finite Quantum Well

Boundary Conditions:

$$\psi(x)|_{x=a,0} \ continous$$

$$\psi'(x)|_{x=a,0} \ continous$$

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



$for\ x < 0, x > a$

$$\boxed{\psi(x) = Ae^{-jk_1x} + Be^{jk_1x}} \qquad k_1 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

$for\ 0 \le x \le a$

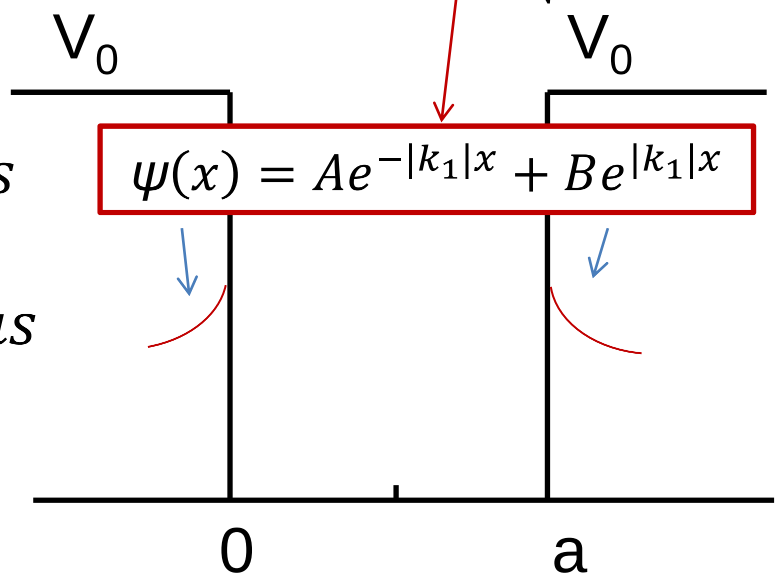
$$\boxed{\psi(x) = Ce^{-jk_2x} + De^{jk_2x}} \qquad k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$

Electrons in Finite Quantum Well

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

Boundary Conditions:

$$\boxed{\psi(x) = Ae^{-|k_1|x} + Be^{|k_1|x}}$$



$$\psi(x)|_{x=a,0} \ \ continous$$

$$\psi'(x)|_{x=a,0} \ \ continous$$

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

$for\ x < 0, x > a$

$$\boxed{\Psi(x) = Ae^{-jk_1x} + Be^{jk_1x}} \quad k_1 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

$for\ 0 \leq x \leq a$

$$\boxed{\Psi(x) = Ce^{-jk_2x} + De^{jk_2x}} \quad k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$

Electrons in Finite Quantum Well

Boundary Conditions:

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

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

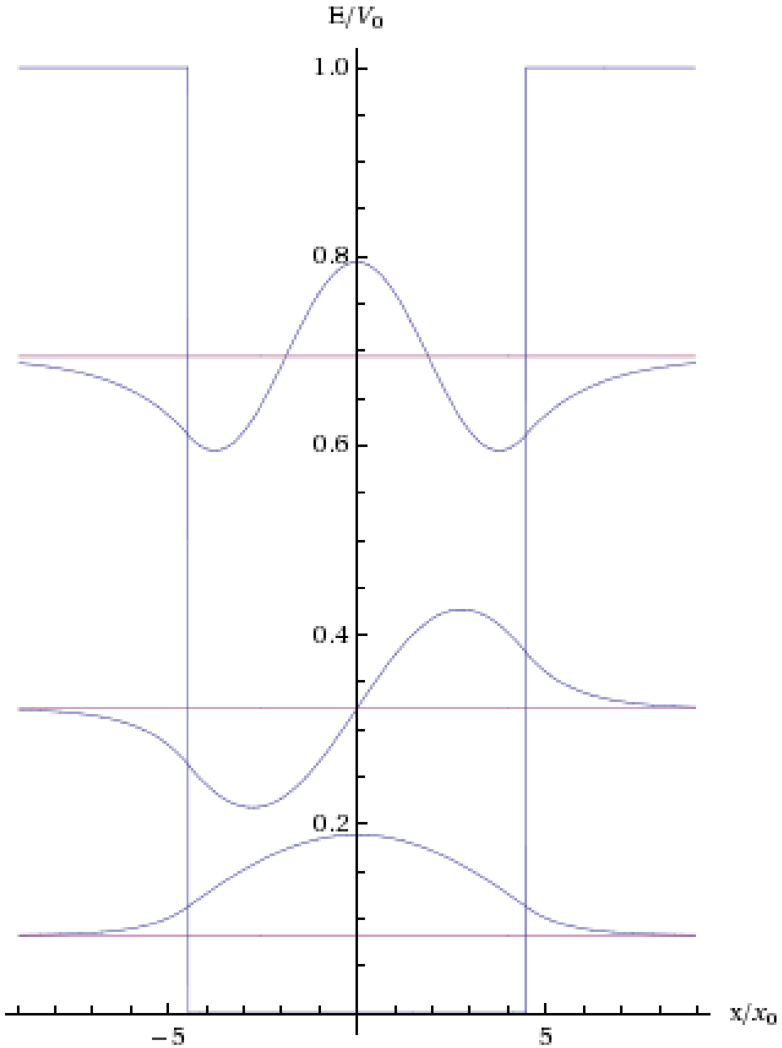
$$\int_{-\infty}^{\infty} \psi(x)\psi^*(x)dx = 1$$

$for\, x < 0, x > a$

$$\boxed{\psi(x) = Ae^{-jk_1x} + Be^{jk_1x}}$$

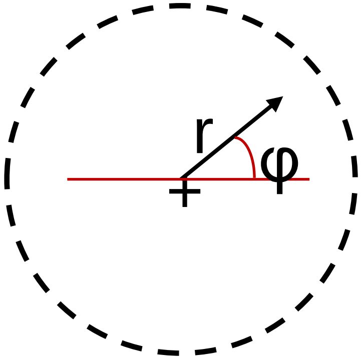
$for\, 0 \leq x \leq a$

$$\boxed{\psi(x) = Ce^{-jk_2x} + De^{jk_2x}}$$

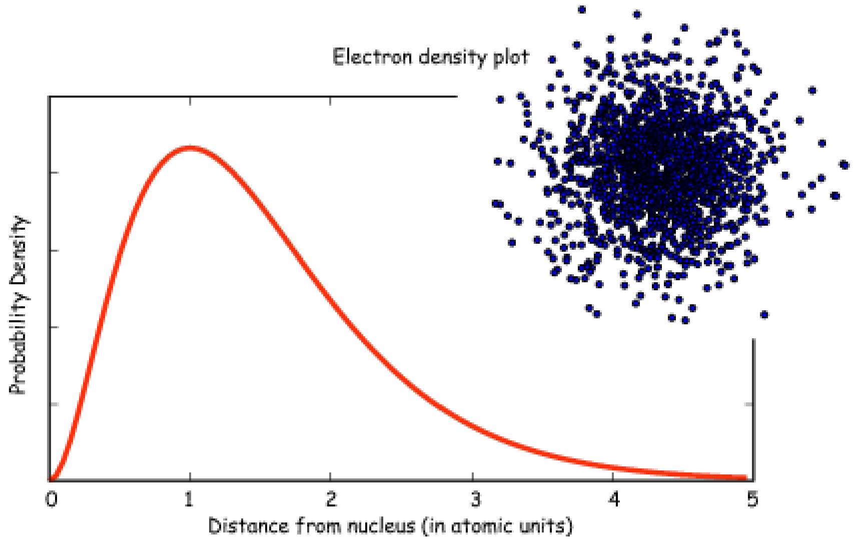


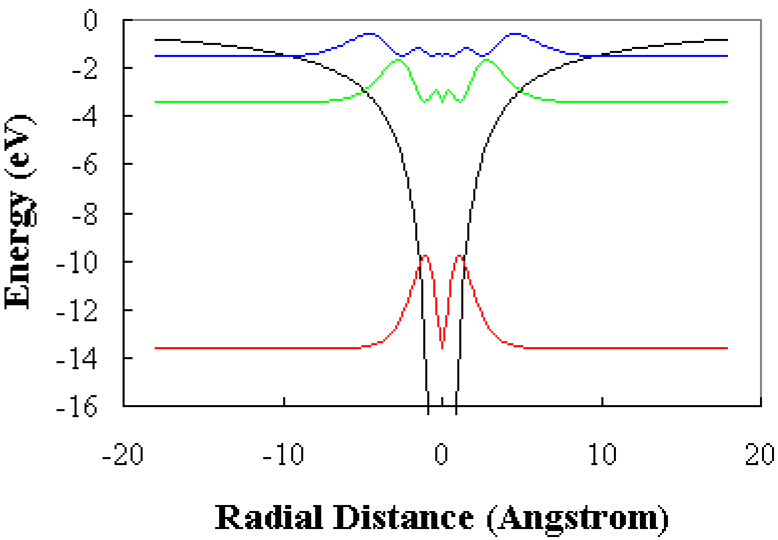
Electrons in Atom

- 2D



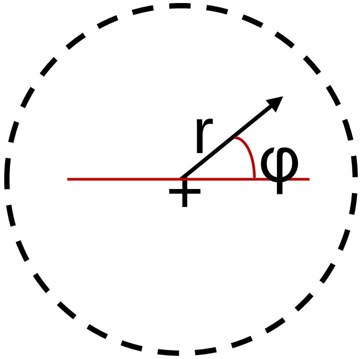
Periodic boundary conditions

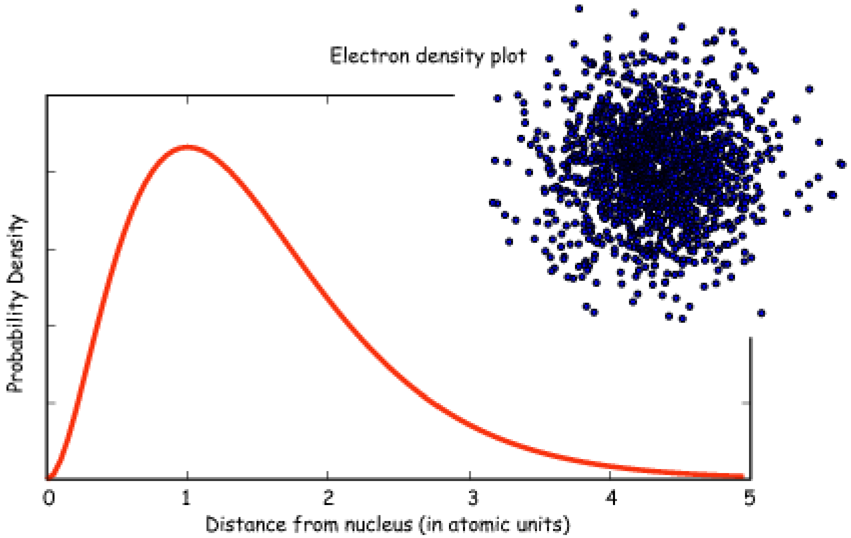




Electrons in Atom

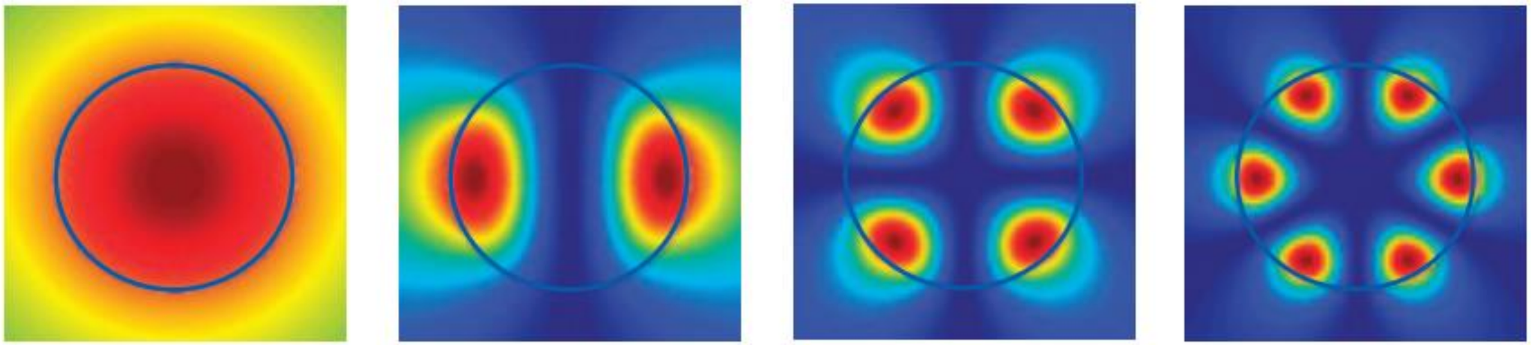
- <u>2D</u>





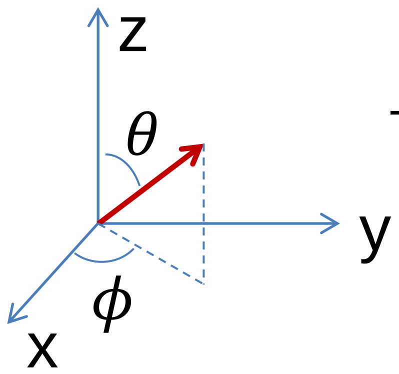
Periodic boundary conditions

f(r, φ)



Electrons in Atom

- <u>3D: one-electron atom</u>



Potential function $V(r) = \dfrac{-e^2}{4\pi\epsilon_0 r}$

Time-independent Schrodinger's wave equation in 3D

$$\nabla^2\psi(r, \theta, \phi) + \frac{2m_0}{\hbar^2}(E - V(r))\psi(r, \theta, \phi) = 0$$

∇^2 is the Laplacian operator

In spherical coordinates,

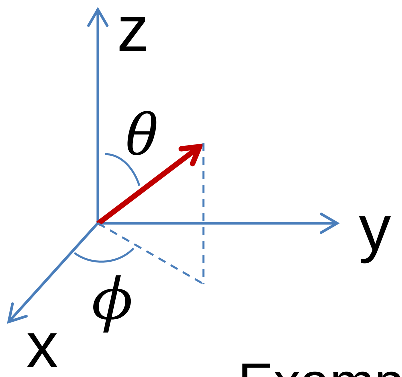
$$\frac{1}{r^2}\cdot\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2\psi}{\partial\phi^2} + \frac{1}{r^2\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{\partial\psi}{\partial\theta}\right) + \frac{2m_0}{\hbar^2}(E - V(r))\psi = 0$$

Separation-of-variables again

$$\psi(r, \theta, \phi) = R(r)\cdot\Theta(\theta)\cdot\Phi(\phi)$$

Electrons in Atom

- <u>3D: one-electron atom</u>



Equation becomes

$$\frac{\sin^2\theta}{R}\cdot\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{1}{\Phi}\cdot\frac{\partial^2\phi}{\partial\phi^2}+\frac{\sin\theta}{\Theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{\partial\Theta}{\partial\theta}\right)$$
$$+r^2\sin^2\theta\cdot\frac{2m_0}{\hbar^2}(E-V)=0$$

Example of solution: second term is equal to a constant

$$\frac{1}{\Phi}\cdot\frac{\partial^2\Phi}{\partial\phi^2}=-m^2$$

Solution: $\phi = e^{jm\phi}$

Wave function must be single-valued, so $\Phi(\phi)=\Phi(\phi+2\pi)$

Then $m = 0, \pm1, \pm2, \pm3, \ldots$

Electrons in Atom

- <u>3D: one-electron atom</u>

The separation-of-variables constants n, l, and m are known as *quantum numbers* .
n: principal quantum number,
l: azimuthal or angular quantum number,
m: magnetic quantum number.
The quantum numbers are related by
n = 1, 2, 3, . . .
l = n-1, n-2, n-3, . . . 0
|m| = *l*, *l*-1, . . . , 0

- Electron energy $$E_n = \frac{-m_0 e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2}$$

$$\text{For } n = 1; \quad E_1 = -13.58 \text{ eV}$$

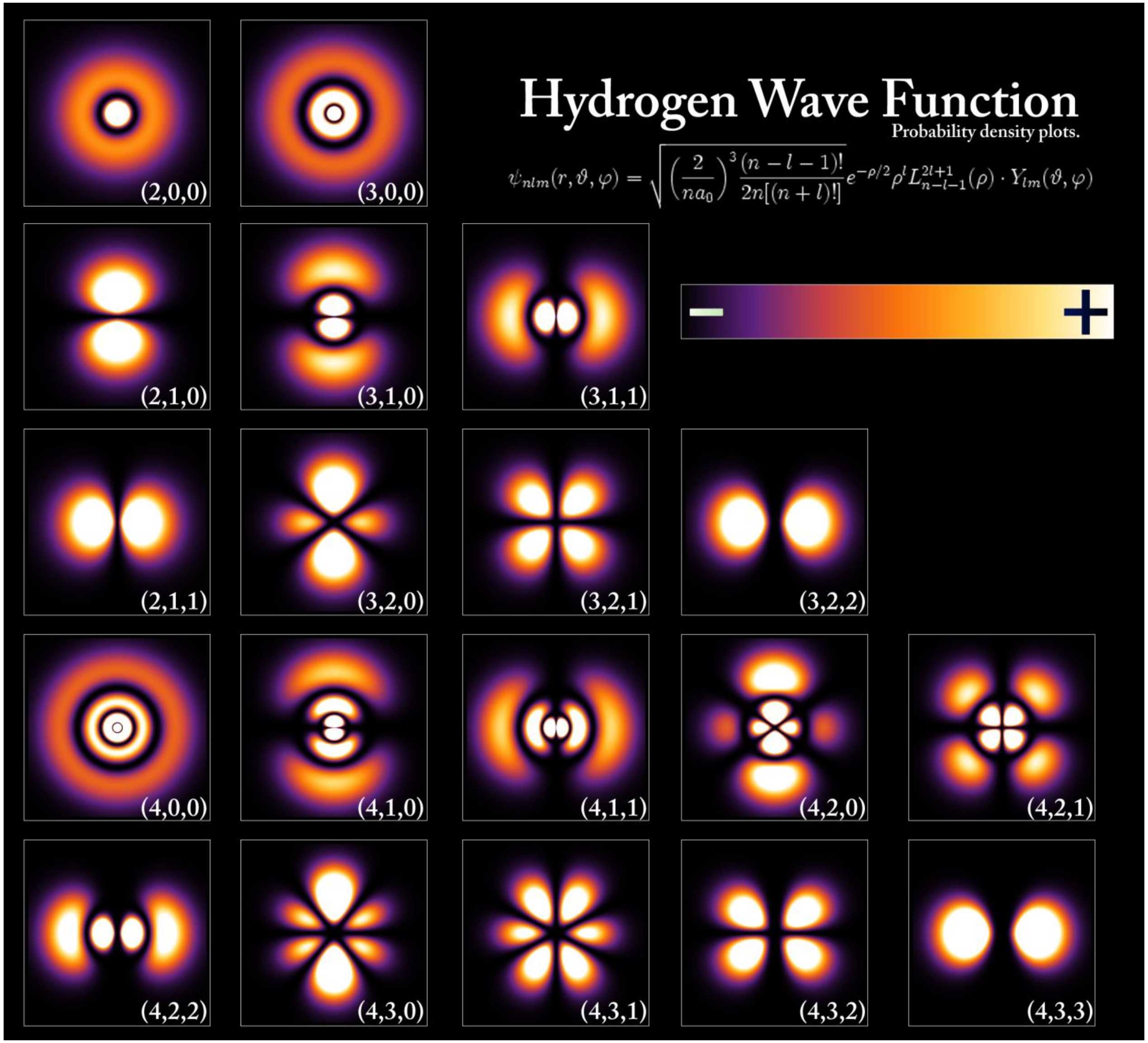
Electrons in Atom

- 3D

3s^{2}3p^{6}3d^6

2s^{2}2p^6

1s^2



Electron cloud

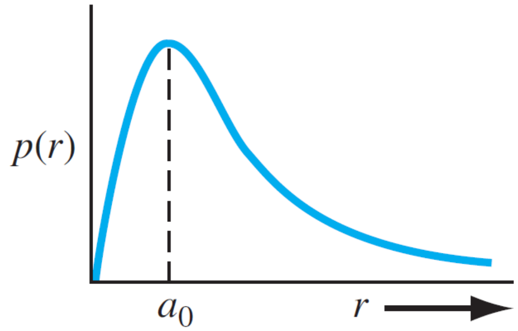
Spin: ½, -½

Pauli exclusion principle: in any given system (an atom, molecule, or crystal), no two electrons may occupy the same quantum state. In an atom, the exclusion principle means that no two electrons may have the same set of quantum numbers.

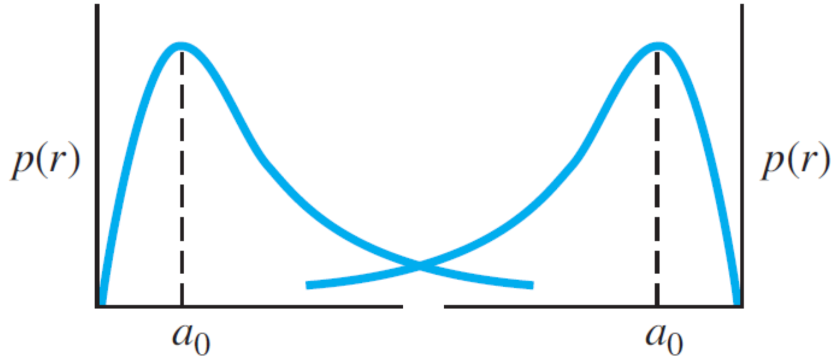
Chapter 3 Quantum Theory of Solids

Energy band

Radial probability density function for the lowest electron energy state of the single, noninteracting hydrogen atom

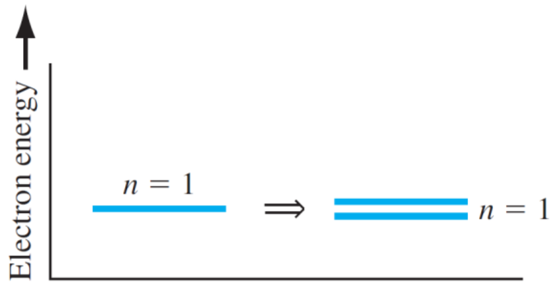


Same probability curves for two atoms that are in close proximity to each other

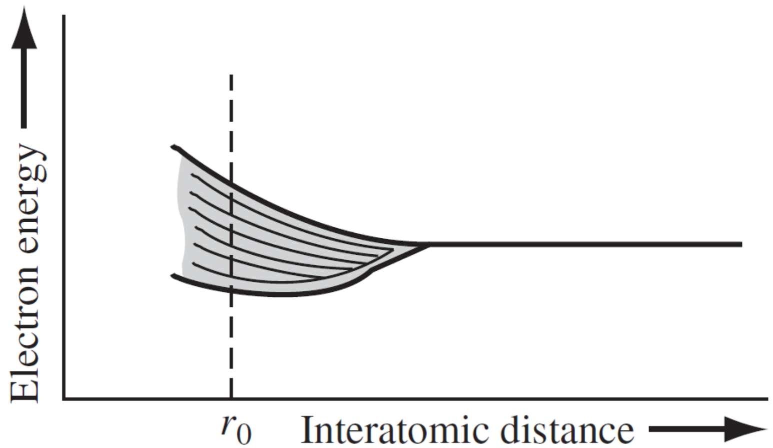


Energy band

Pauli exclusion principle: split into 2 energy levels

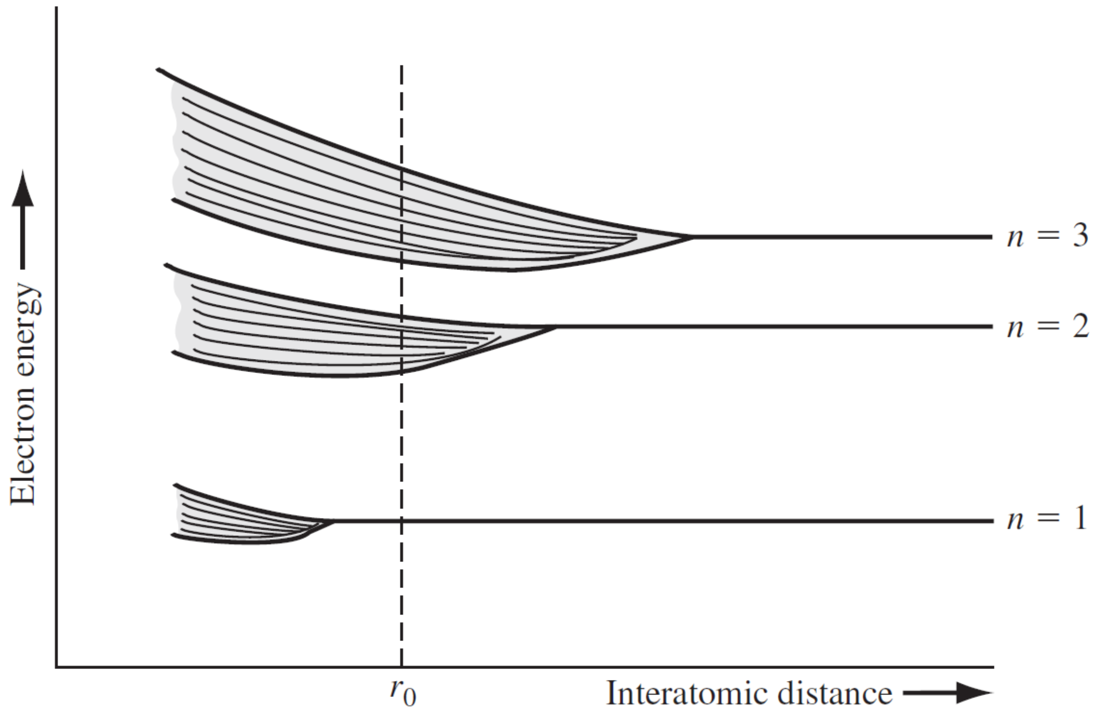


Periodic hydrogen-type atoms: split into an **energy band**



Energy band

Several energy levels: forbidden energies (imaginary crystal)

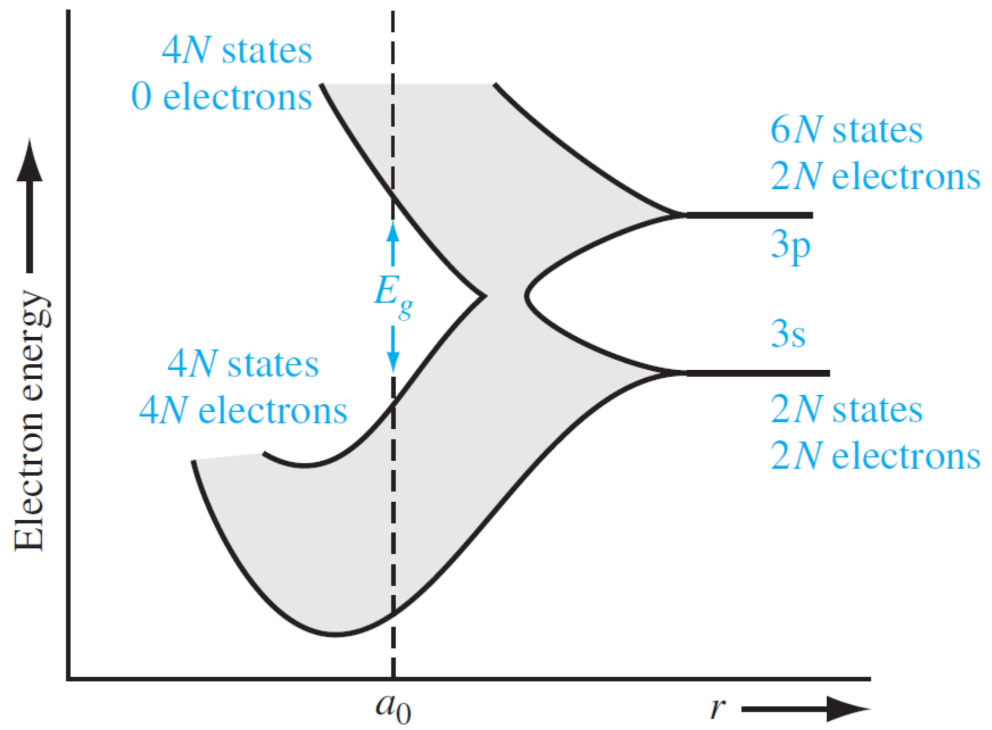


Energy band

Si: real case

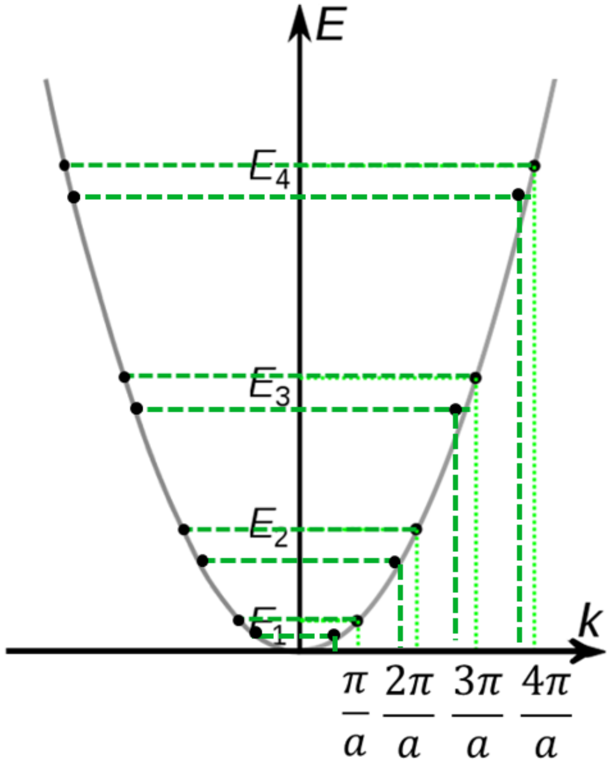
Only valence electrons, n=3 matters

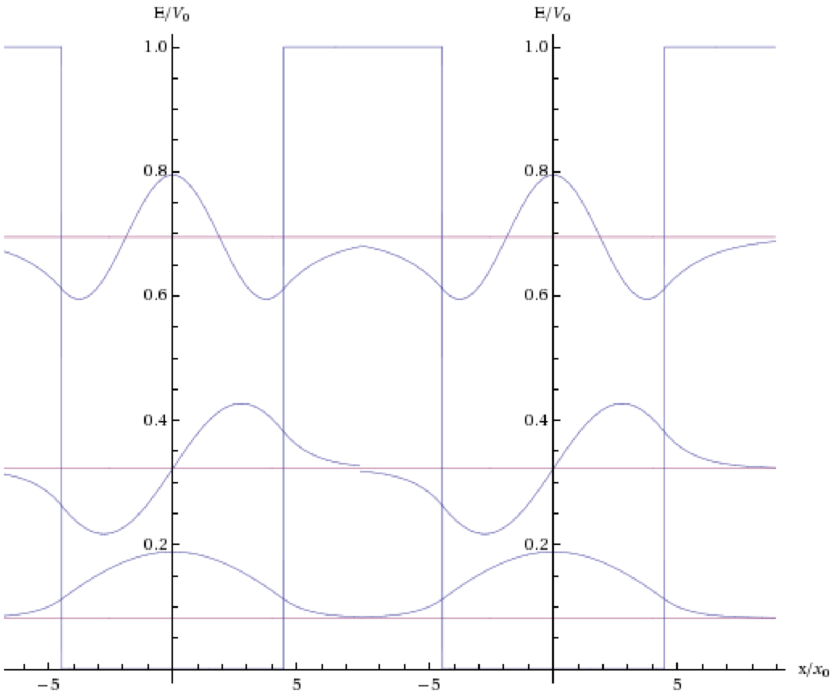
E_g: **band gap**



Electrons in Periodic Finite Quantum Wells

Kronig-Penny Model

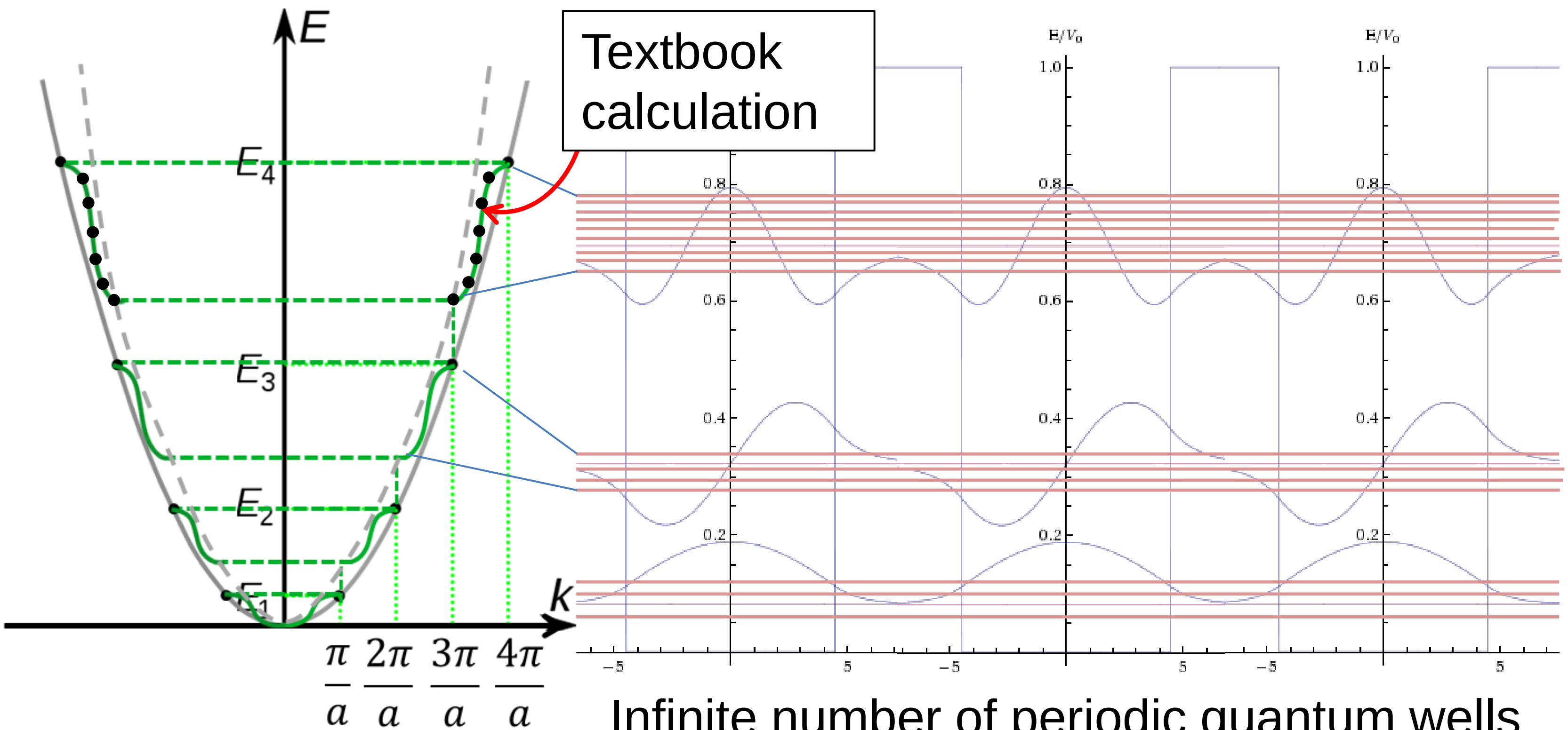




2 quantum wells

Electrons in Periodic Finite Quantum Wells

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



Infinite number of periodic quantum wells

$$\frac{mV_0 ba}{\hbar^2}\frac{sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka)$$

On P.67 eq.(3.22)

Electrons in Periodic Finite Quantum Wells

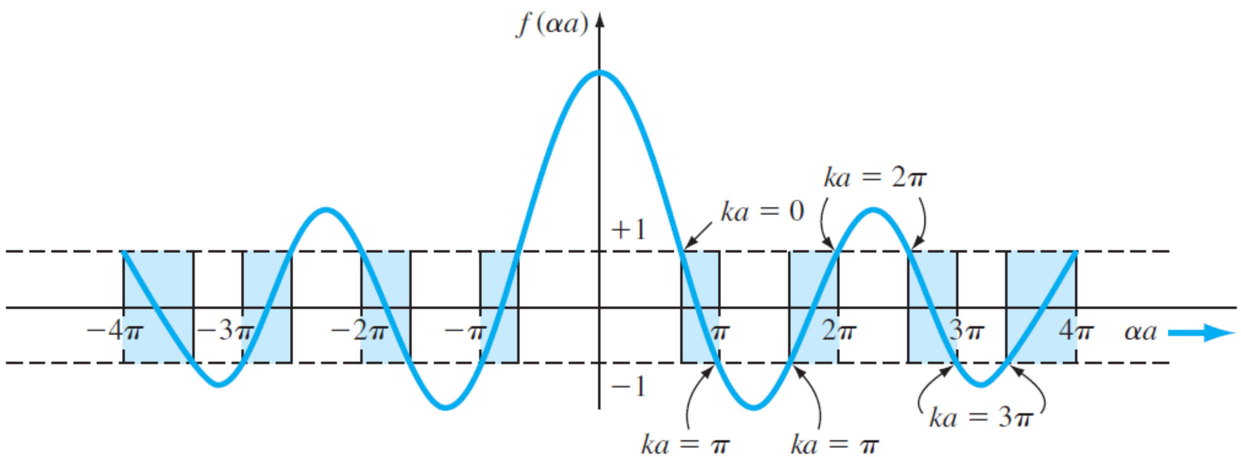
Band structure in physical and k space for 1D periodic quantum wells

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

$$P' = \frac{mV_0ba}{\hbar^2}$$

$$P'\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

Define $f(\alpha a) = P'\frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ between +1 and -1

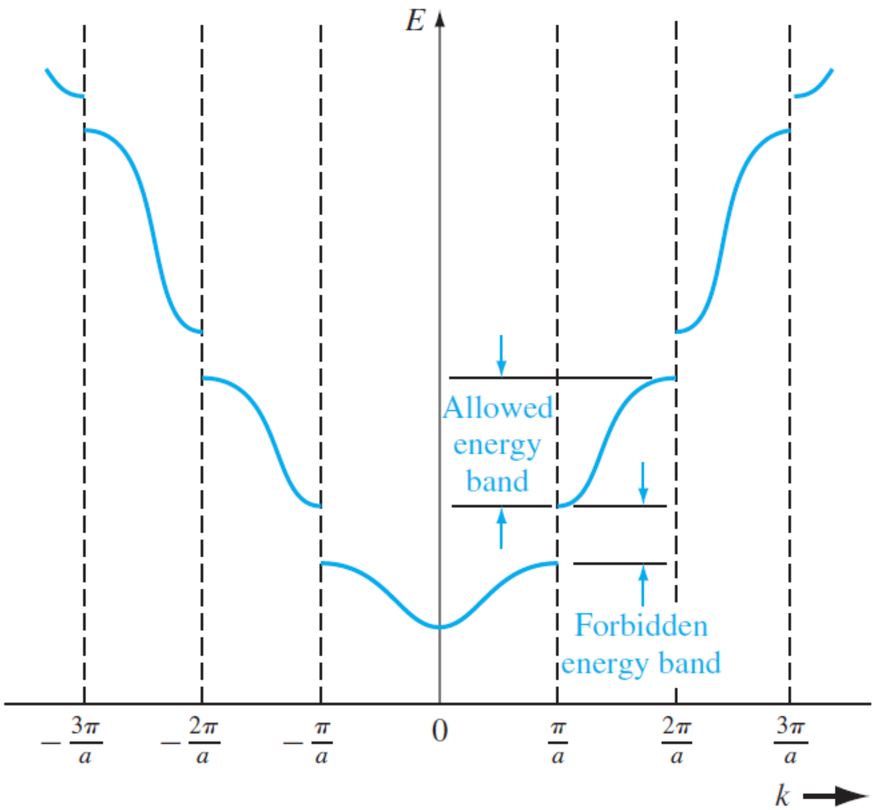


Electrons in Periodic Finite Quantum Wells

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

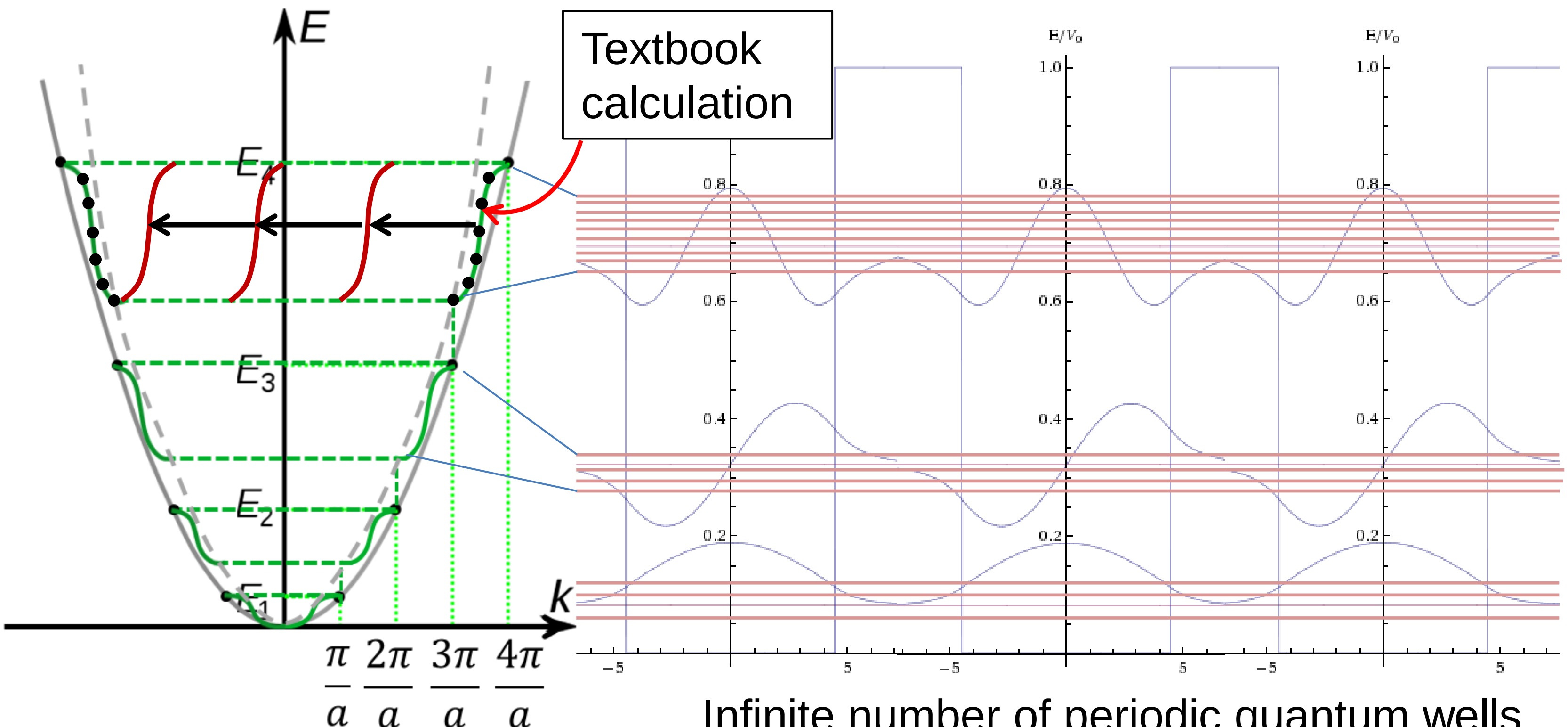
$$\alpha^2 = \frac{2mE}{\hbar^2}$$

Allowed energy bands:



Electrons in Periodic Finite Quantum Wells

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

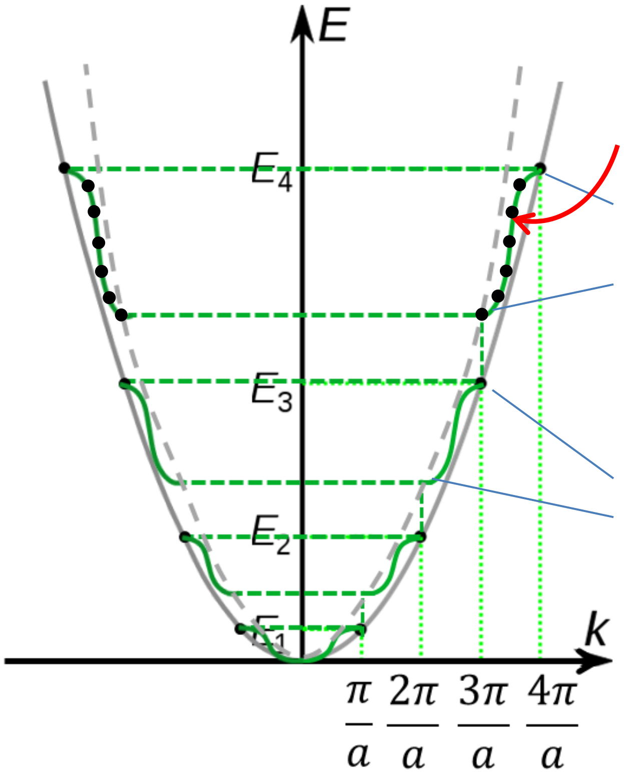


Infinite number of periodic quantum wells

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

Electrons in Periodic Finite Quantum Wells

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



Online 1D band structure calculator

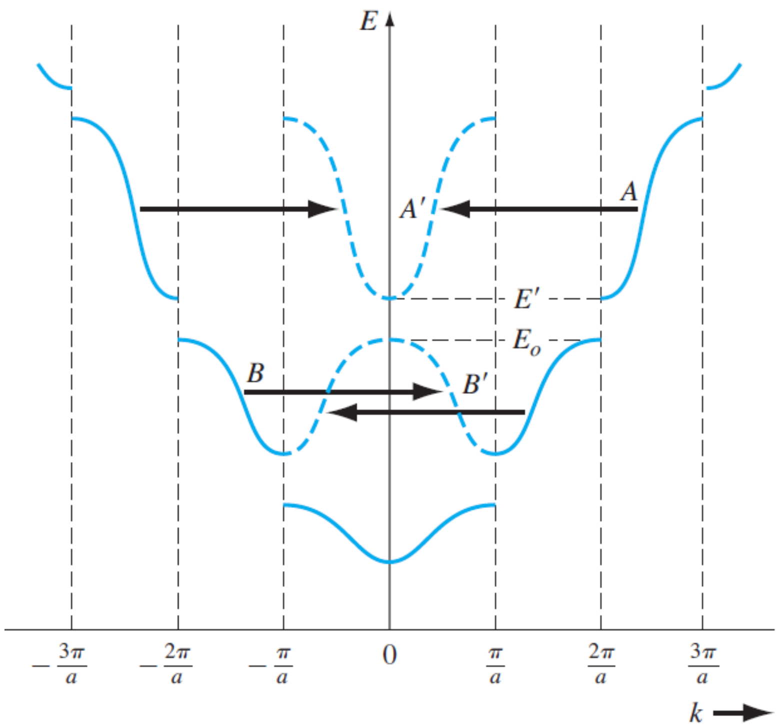
http://lamp.tu-graz.ac.at/~hadley/ss1/bloch/bloch.php

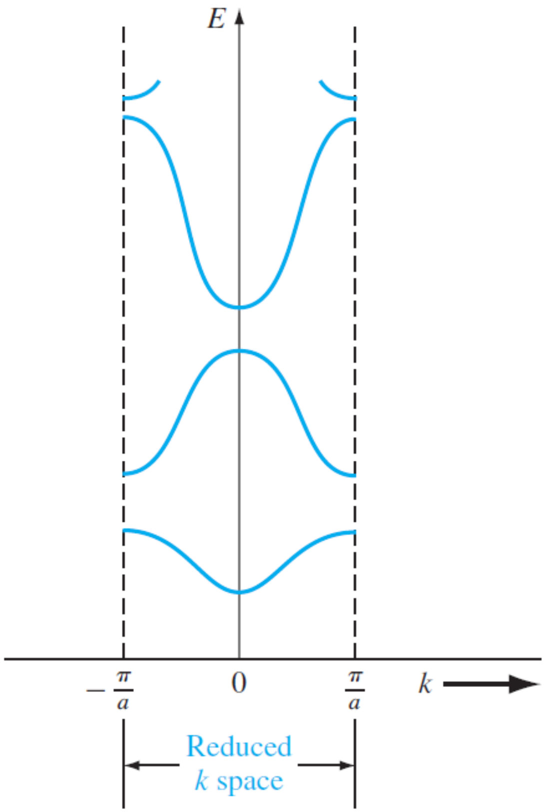
$$\boxed{\frac{mV_0ba}{\hbar^2}\frac{sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka)}$$

Electrons in Periodic Finite Quantum Wells

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

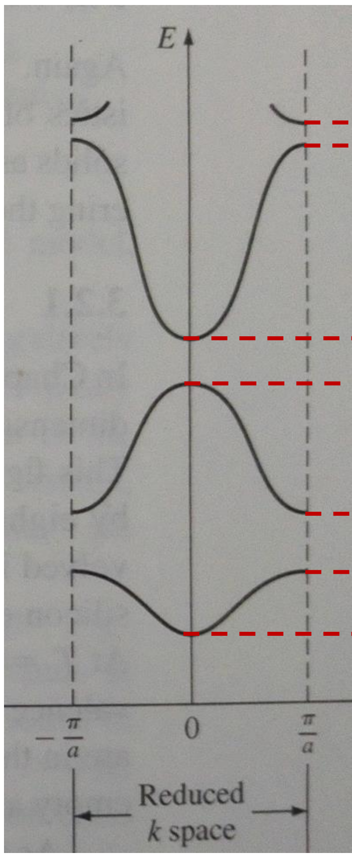
$$\cos ka = \cos(ka + 2n\pi) = \cos(ka - 2n\pi)$$



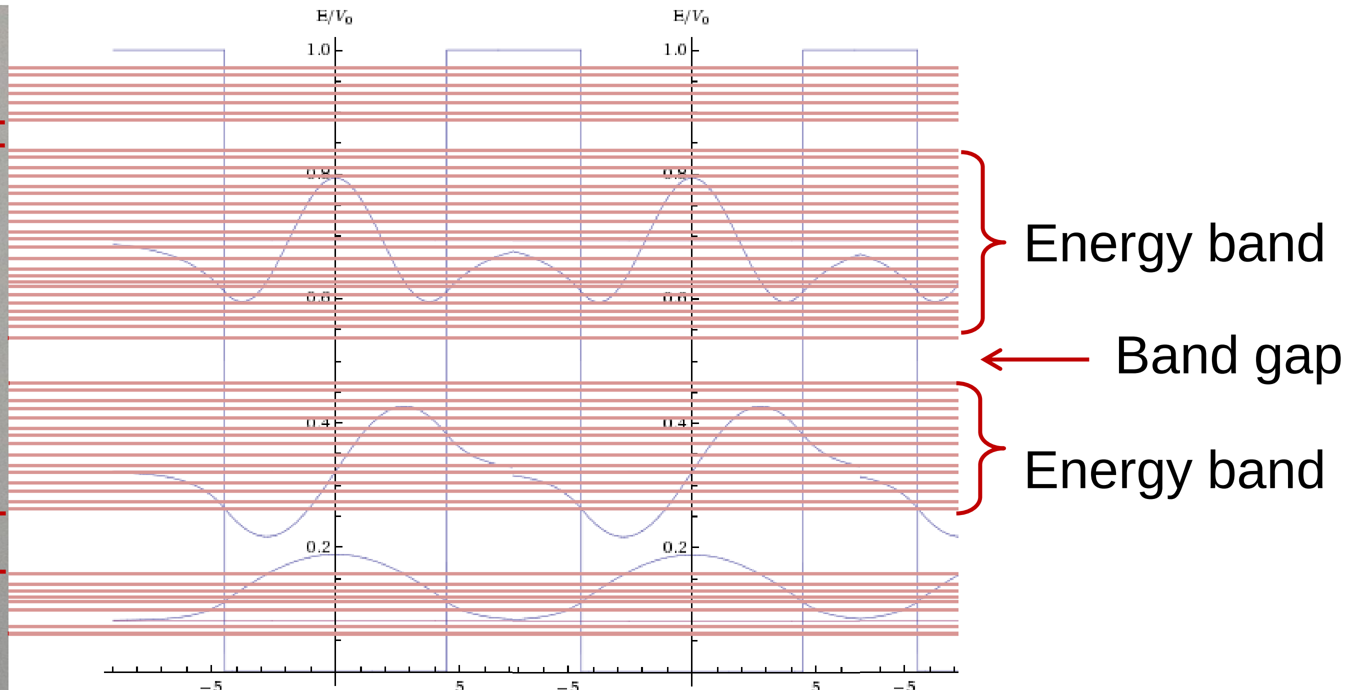


Electrons in Periodic Finite Quantum Wells

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

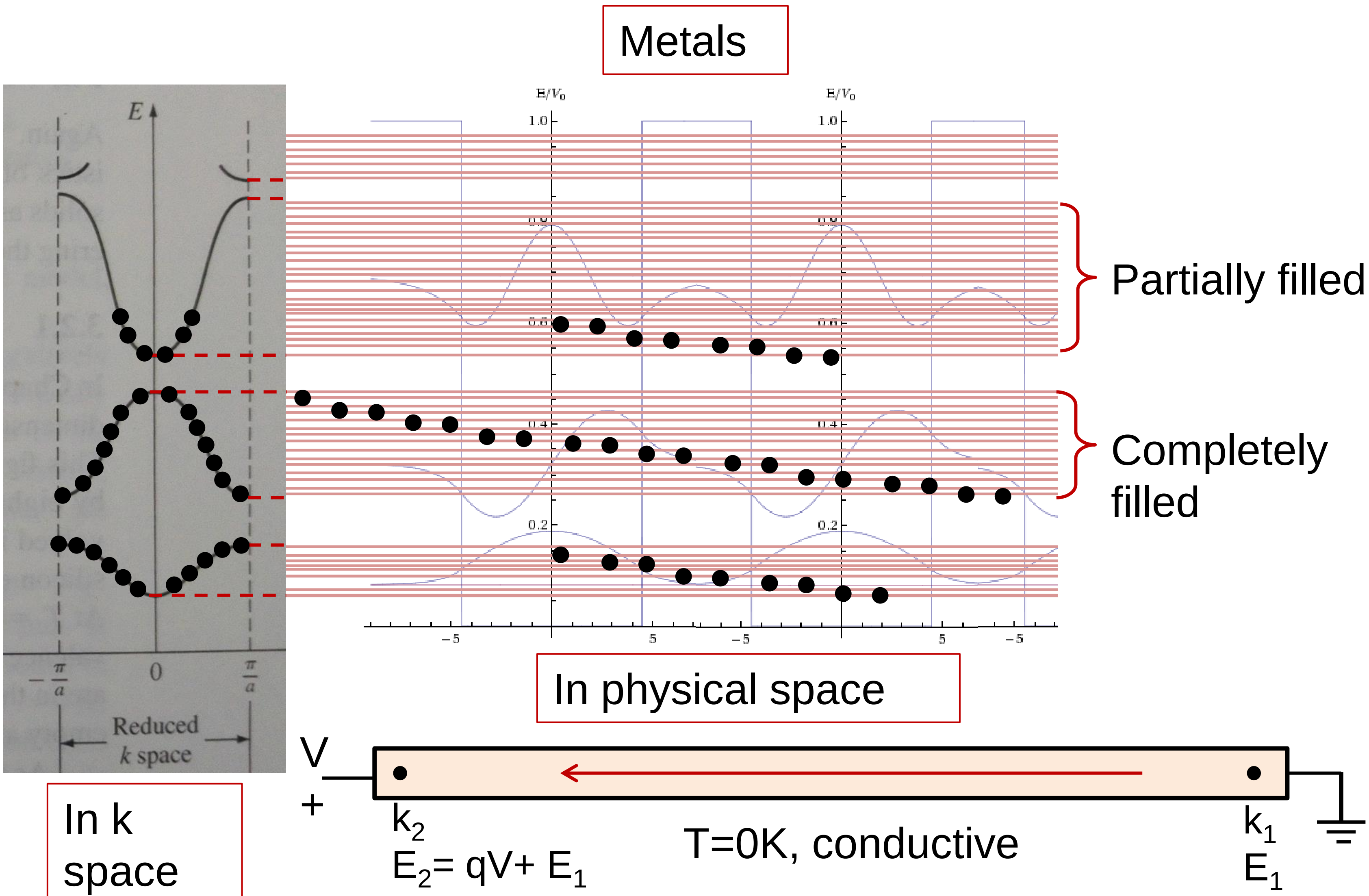


In k space

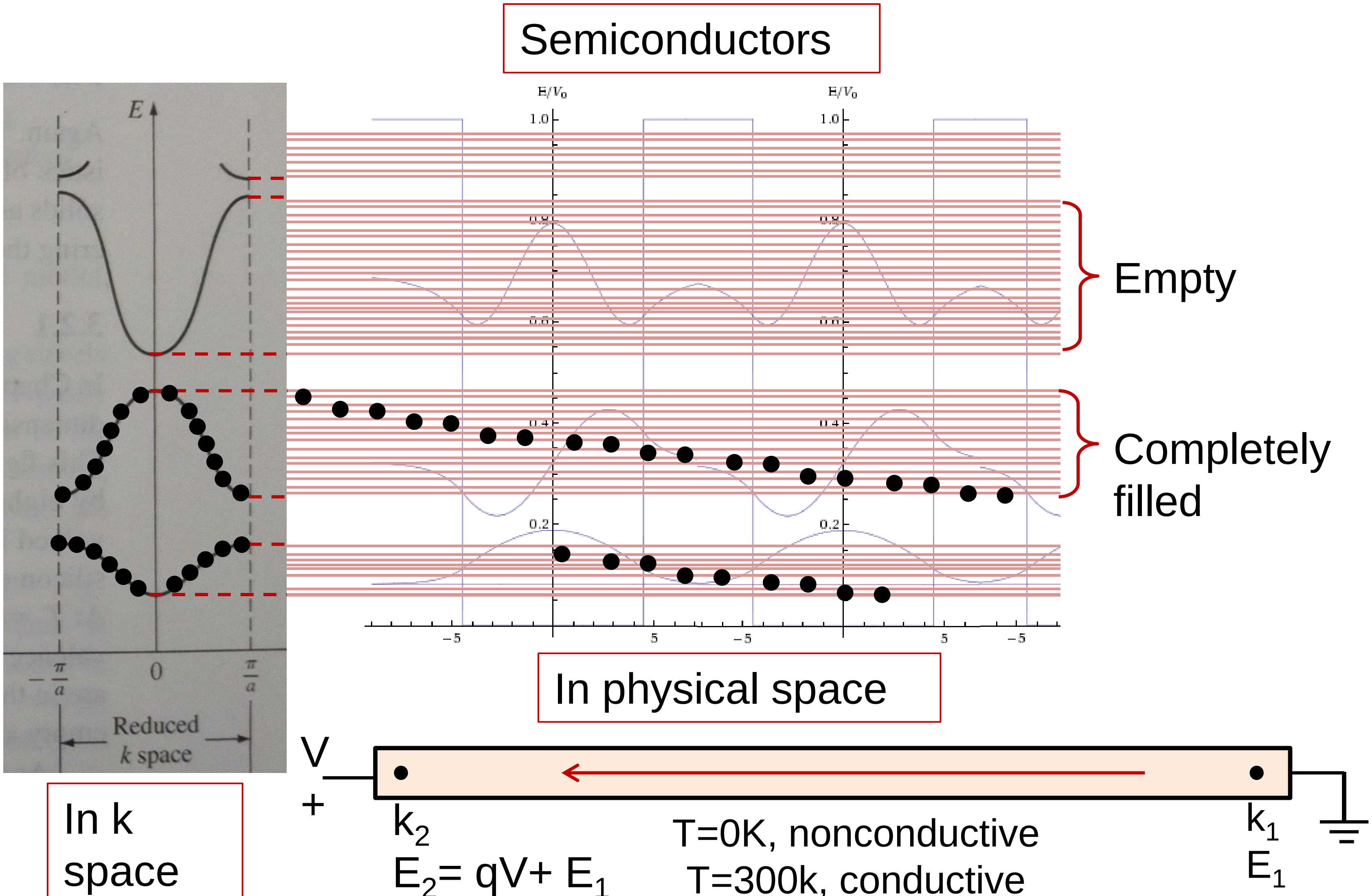


In physical space

Band structures of metals, semiconductors and insulators

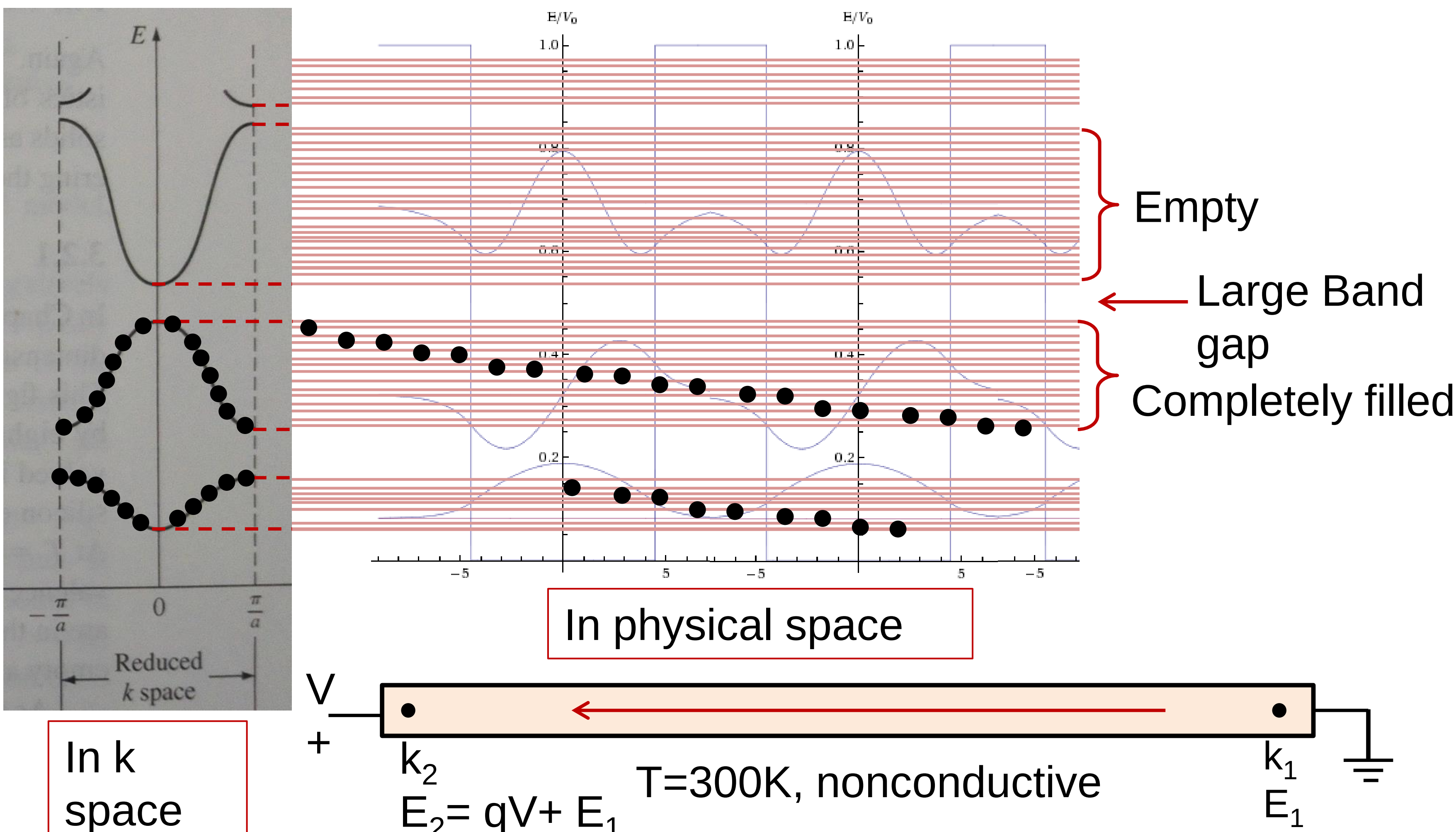


Band structures of metals, semiconductors and insulators



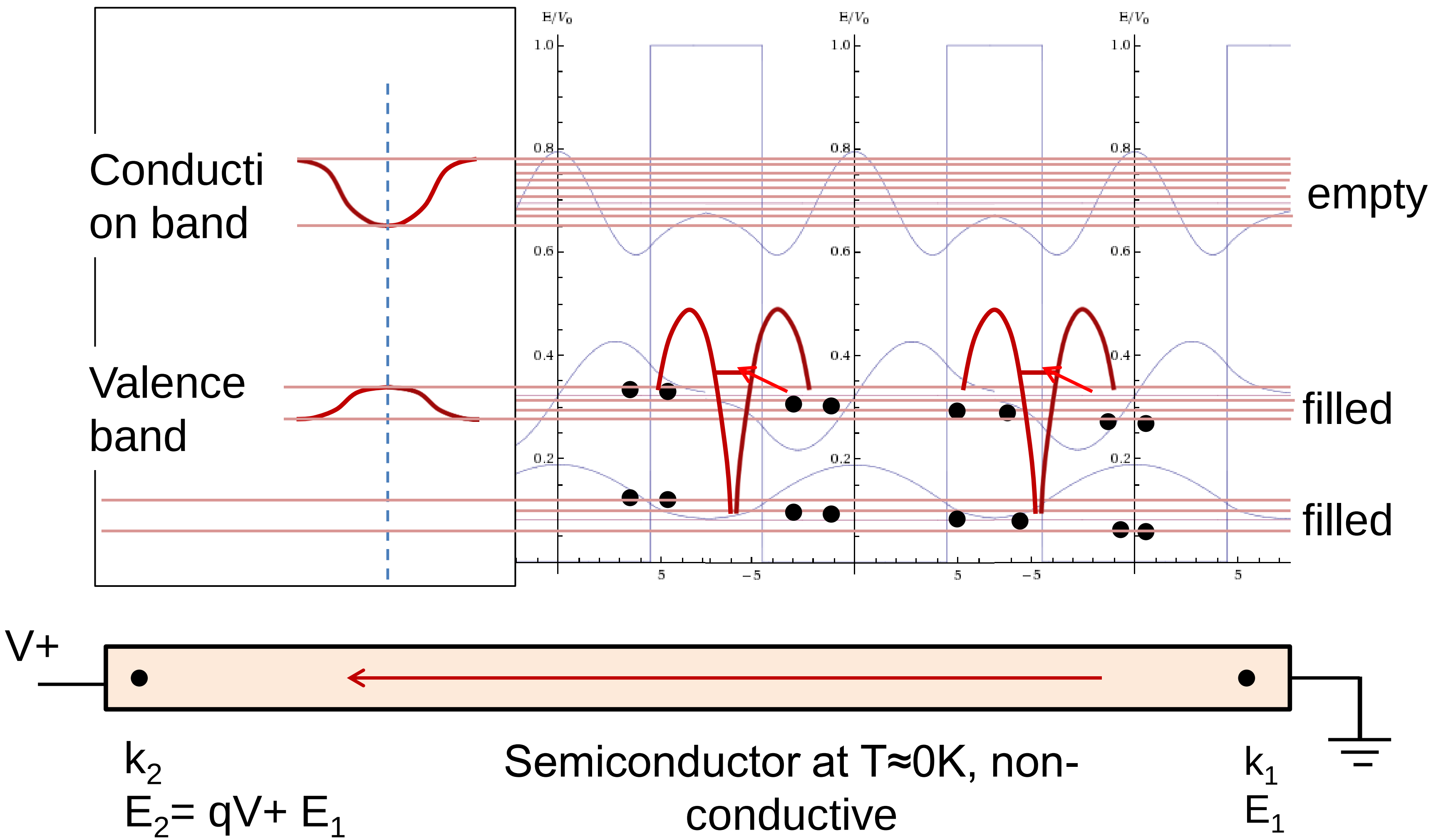
Band structures of metals, semiconductors and insulators

Insulators are wide bandgap semiconductors



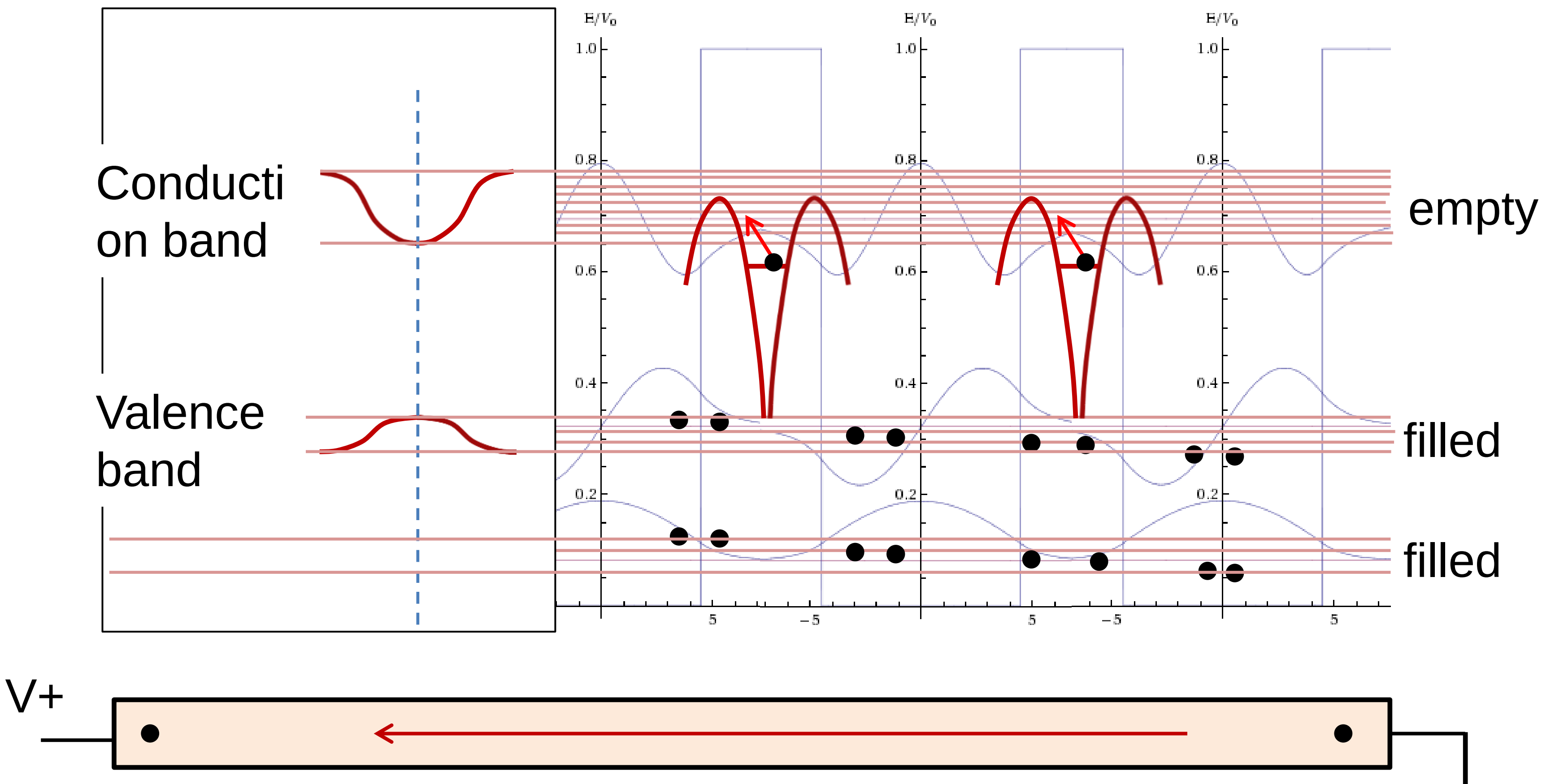
Doping in semiconductors

p-type doping



Doping in semiconductors

n-type doping



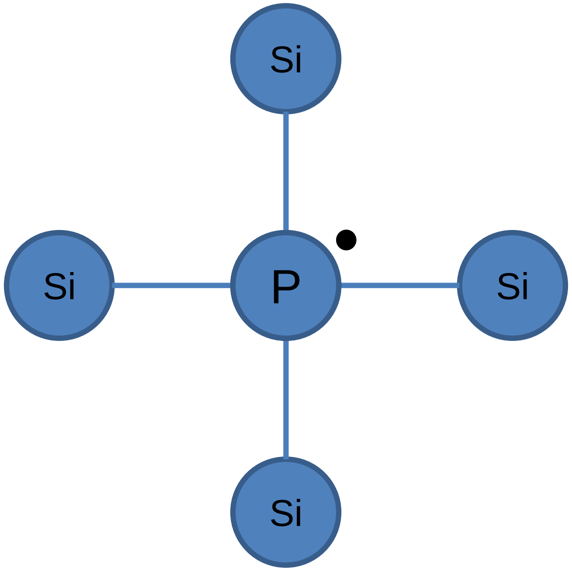
k_2
E_2= qV+ E_1

Semiconductor at T≈0K, non-conductive

k_1
E_1

Doping in semiconductors

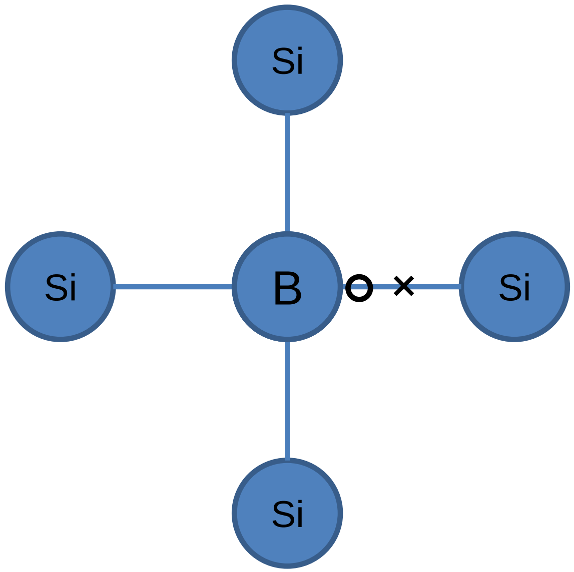
1. n-type, p-type



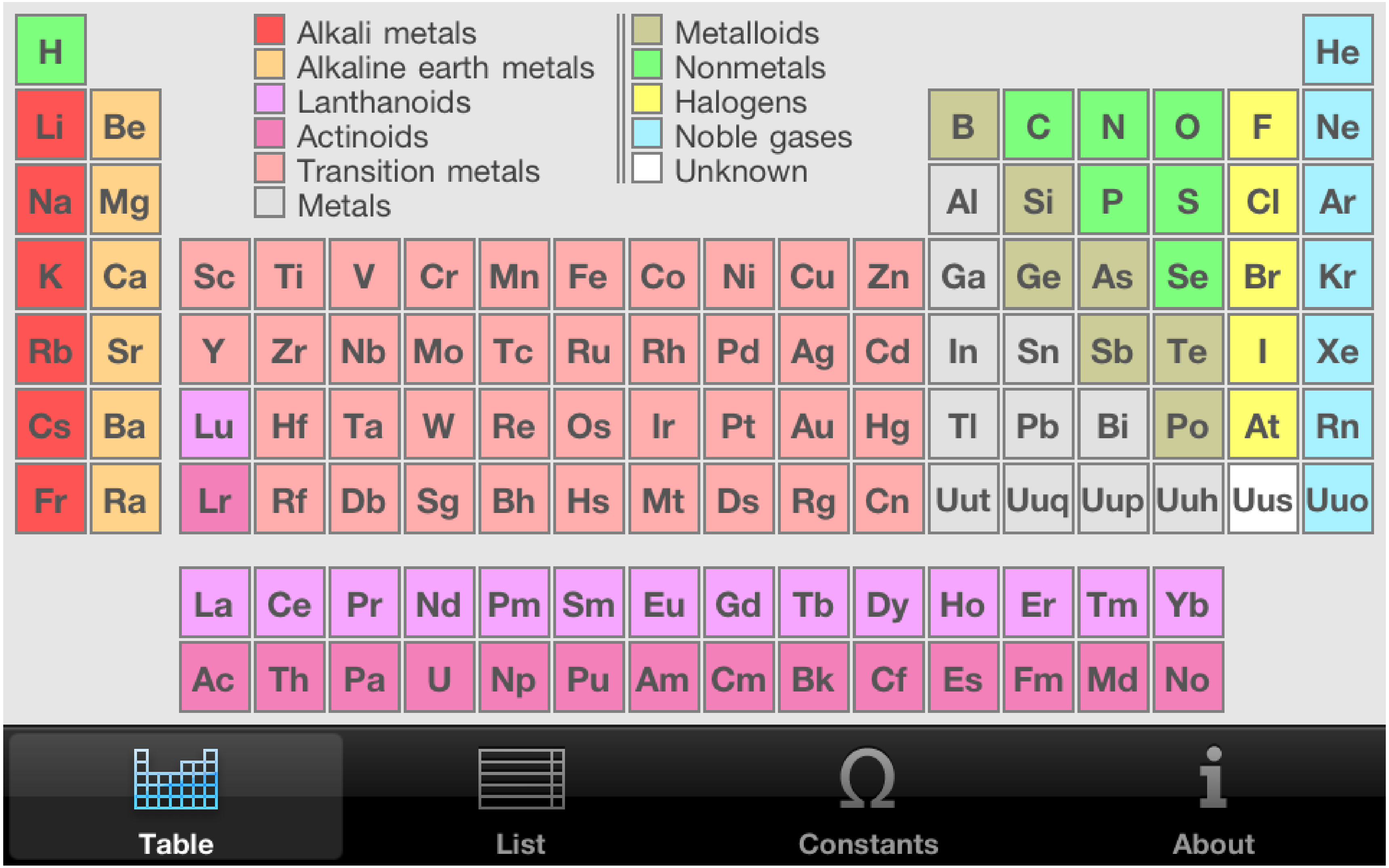
Doping in semiconductors

Two conditions:

- Adjacent group in periodic table
- Chemical bond



Doping in semiconductors



Doping in semiconductors

Two conditions:

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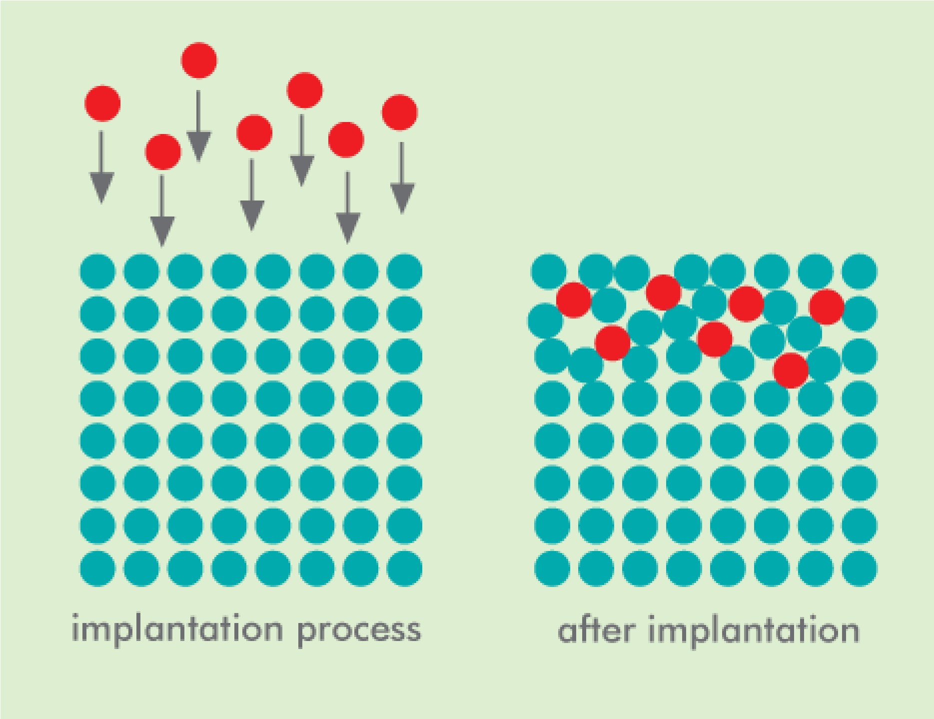

High temperature
Annealing (~900C)
Doping atoms
substitute lattice atoms

doping