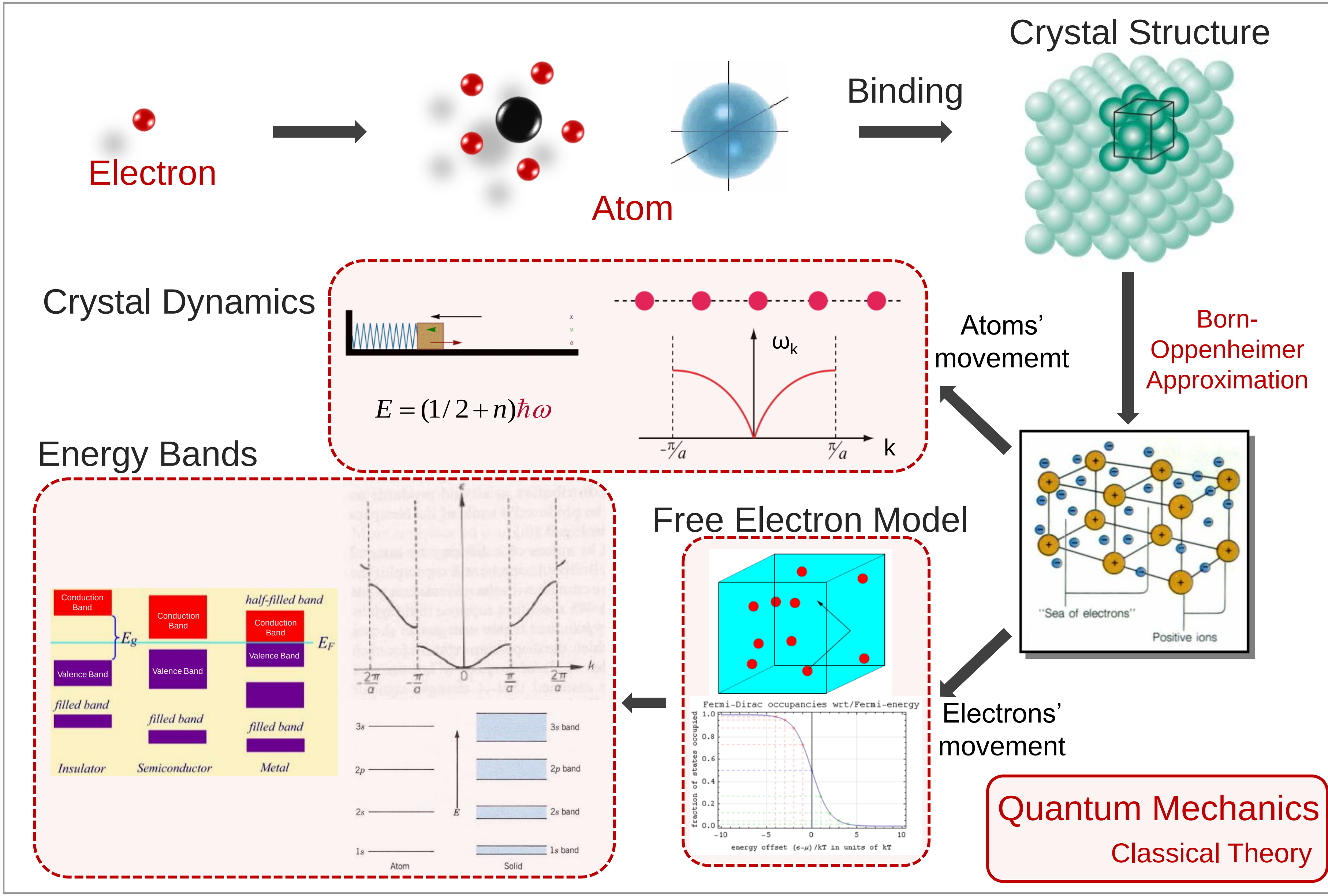
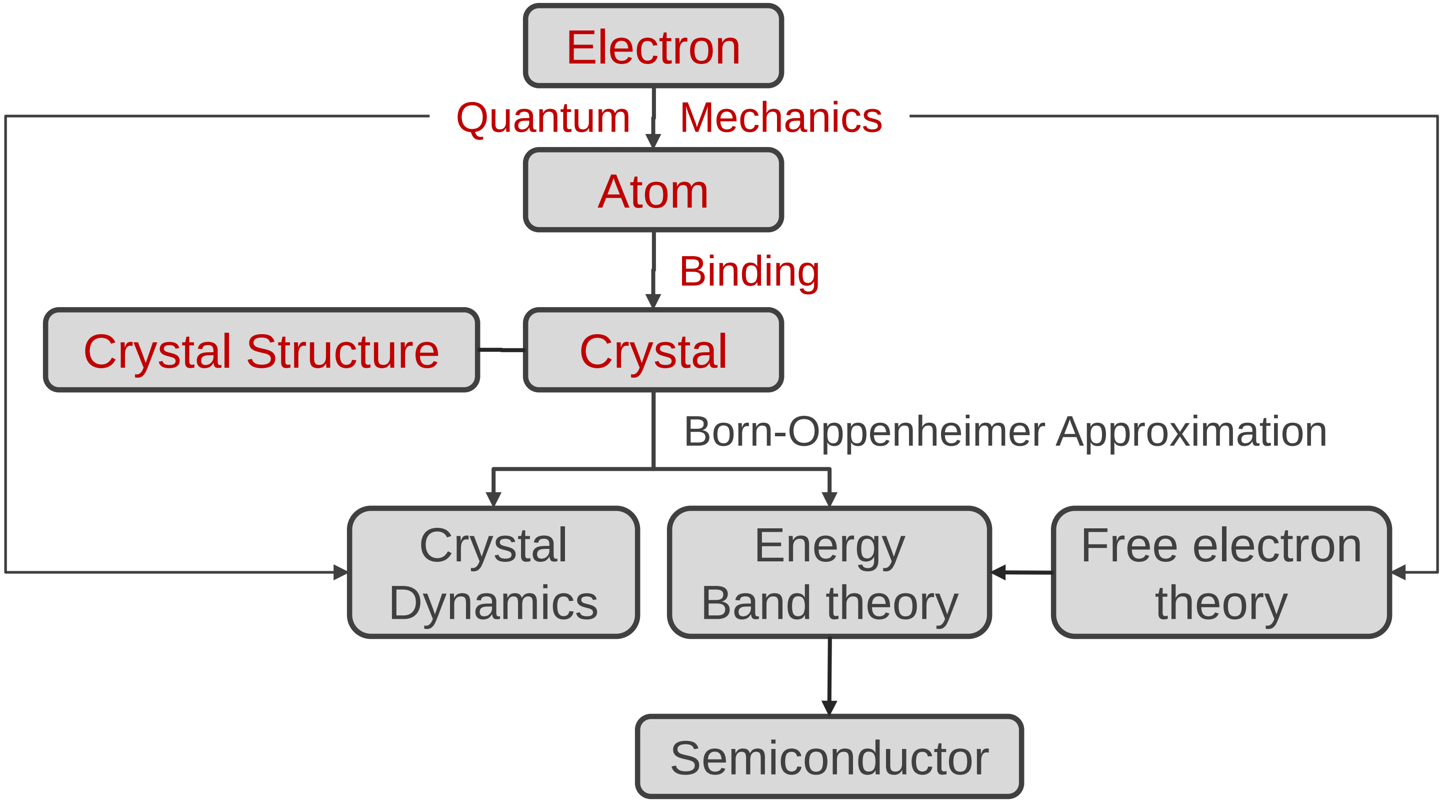
Chapter 1

Formation of Crystal

· Contents and roadmap



· Contents and roadmap



Chapter 1 Formation of Crystal

1.1 Quantum Mechanics and atomic structure

- 1.1.1 Electrons
- 1.1.2 Old quantum theory
- 1.1.3 Method of Quantum Mechanics
- 1.1.4 Distributing functions of micro-particles

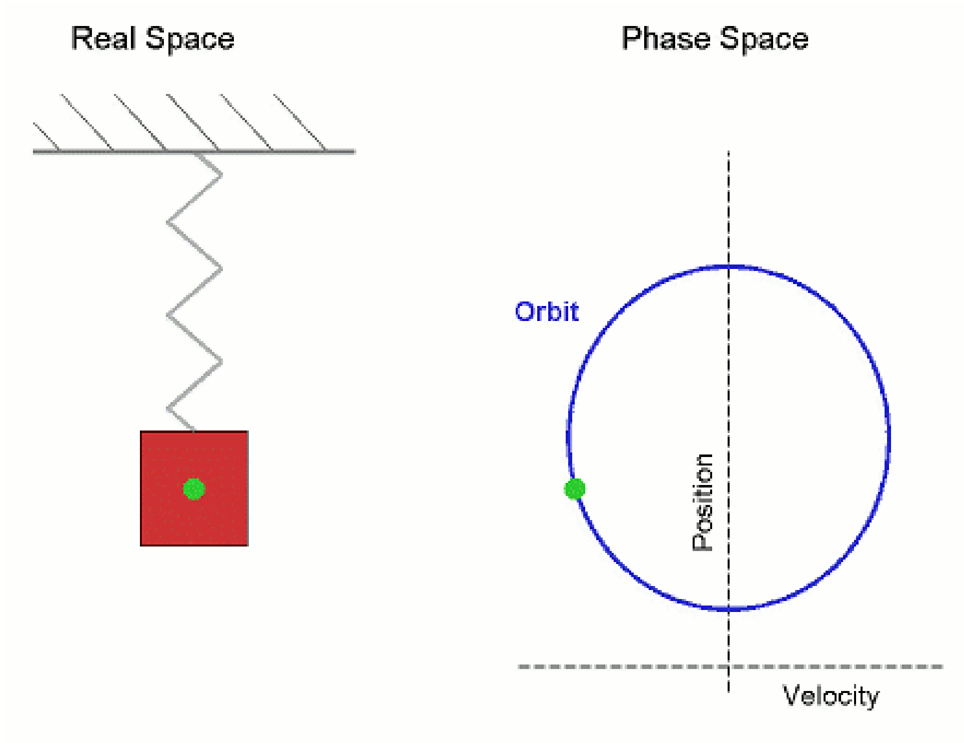
1.2 Binding

1.3 Crystal structure and typical crystals

1.4 Reciprocal Lattice and Brillouin Zone


ATOMIC ENERGY COMMISSION
UNITED STATES OF AMERICA

Problem of planetary model



(1) atom would be unstable
(2) radiate EM wave of continuous frequency

Bohr – Quantum atomic structure
Planck – Quantum

Chapter 1 Formation of Crystal

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1.1.2 Old quantum theory

1.1.3 Method of Quantum Mechanics

1.1.4 Distributing functions of micro-particles

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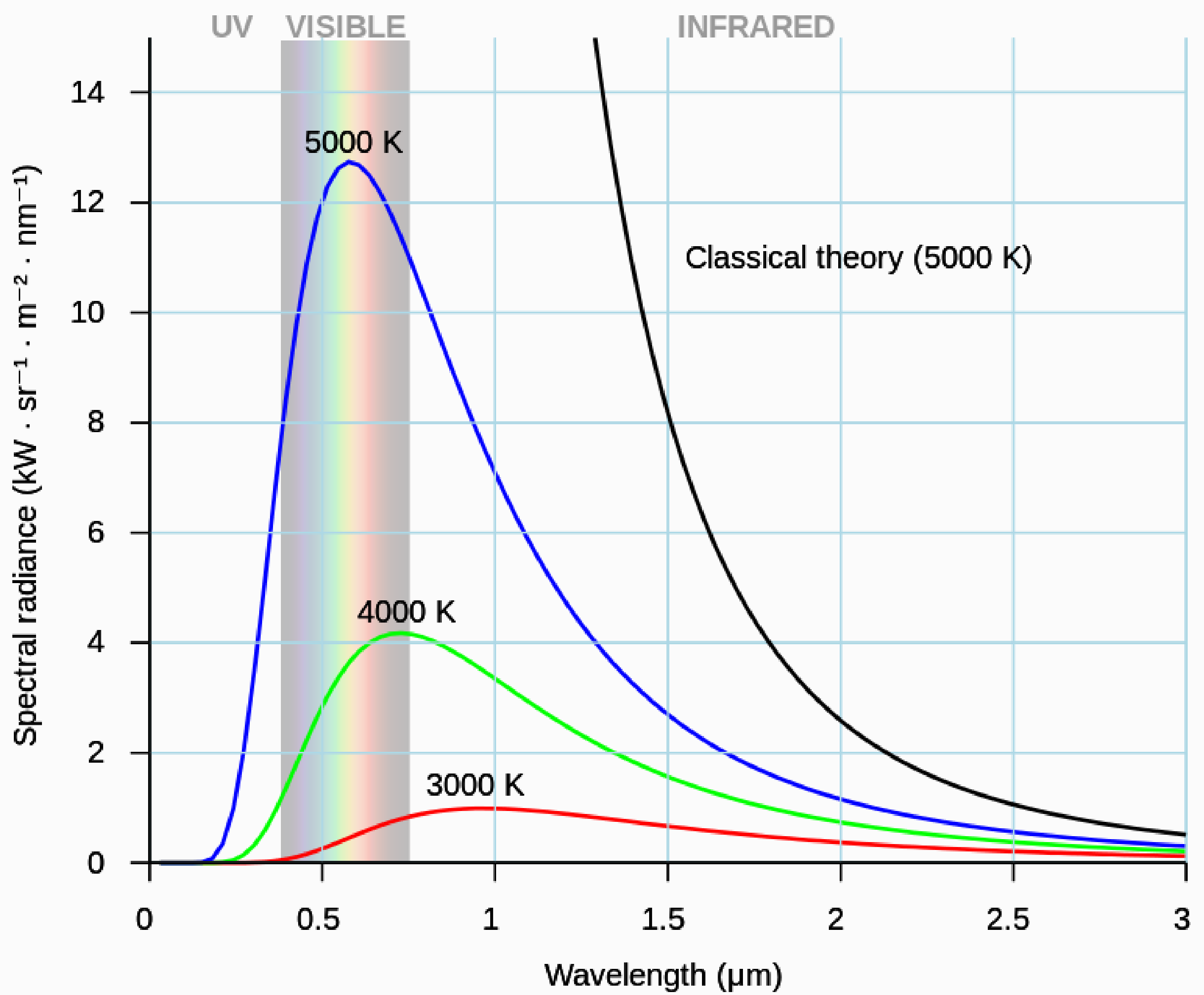
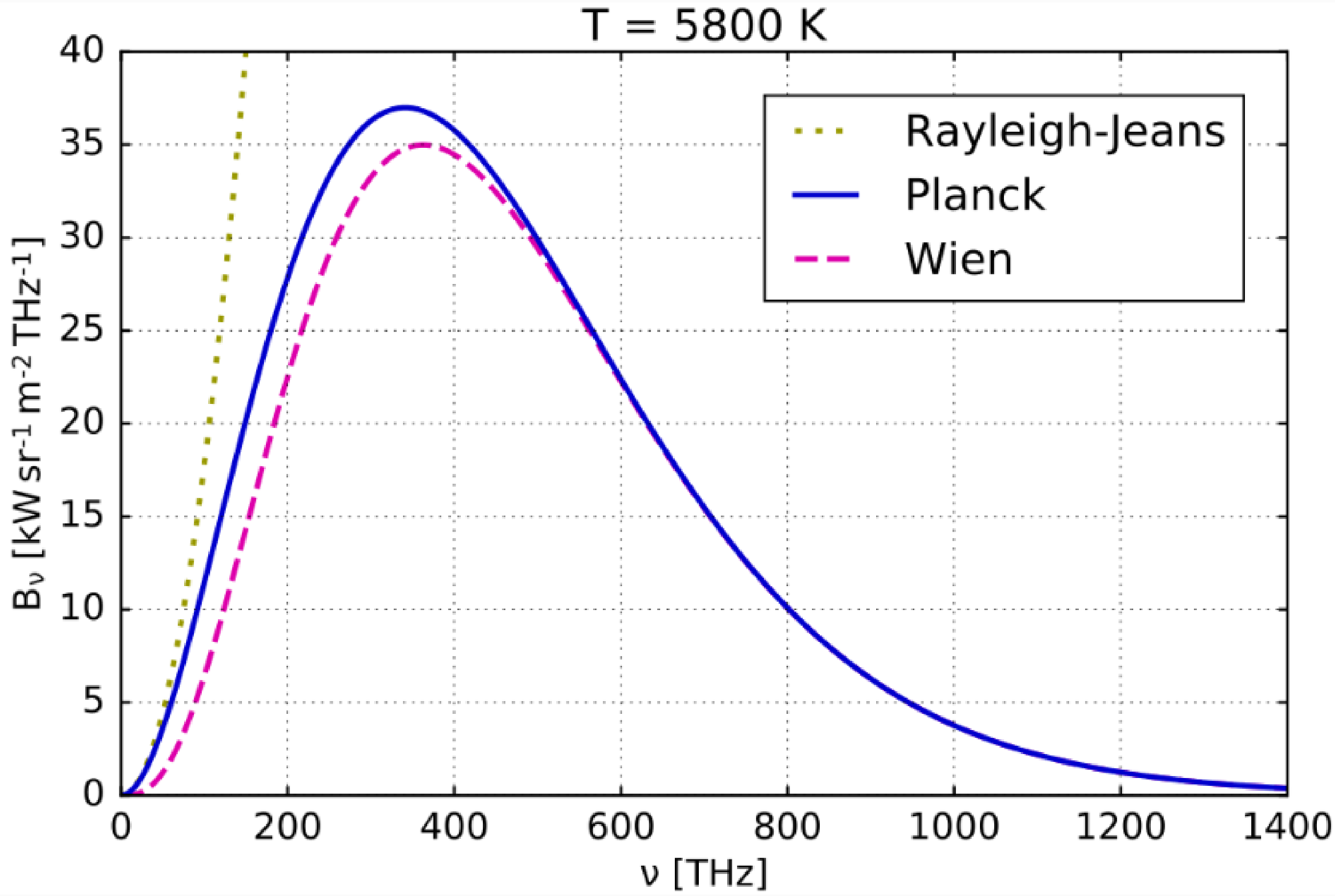
1.4 Reciprocal Lattice and Brillouin Zone

1.5 Defects in Solids



Planck's law accurately describes black body radiation. Shown here are a family of curves for different temperatures. The classical (black) curve diverges from observed intensity at high frequencies. [图片来自维基百科]

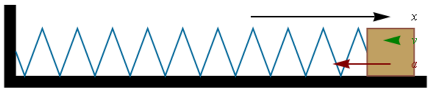


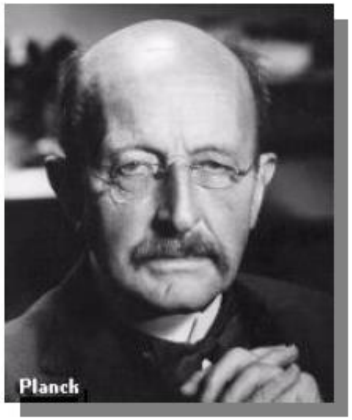
Comparison of Wien's Distribution law with the Rayleigh–Jeans Law and Planck's law, for a body of 5800 K temperature. [图片来自维基百科]

Planck's Theory - 1900

(1) Treat blackbody as large number of atomic oscillators (simple harmonic oscillator), each of which emits and absorbs EM waves

(2) **Each atomic oscillator can have only discrete values of energy**

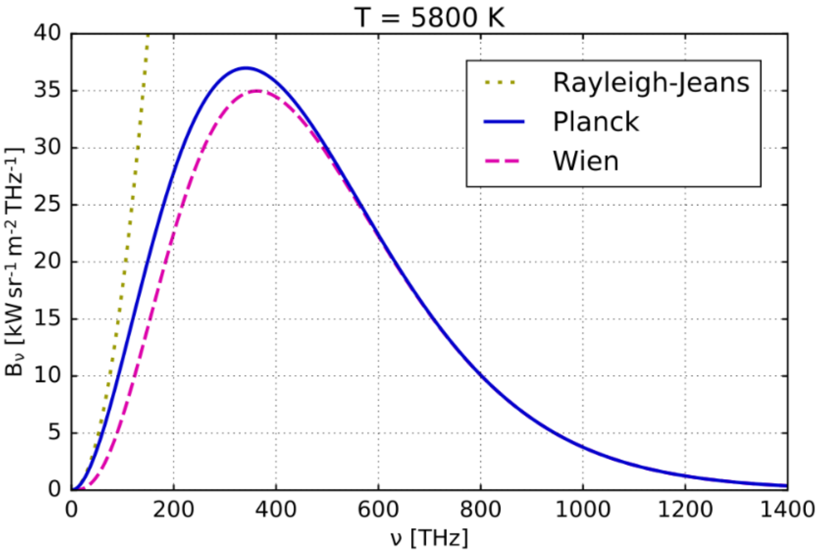




$$E = n\,h\nu\ ,\ n = 0, 1, 2, \ldots$$

h = 6.63 x 10^{-34} J•s (Planck's constant)

(3) The energy of the EM wave emitted by the atomic oscillators must be in multiples of $h\nu$



$h\nu$ -- quanta

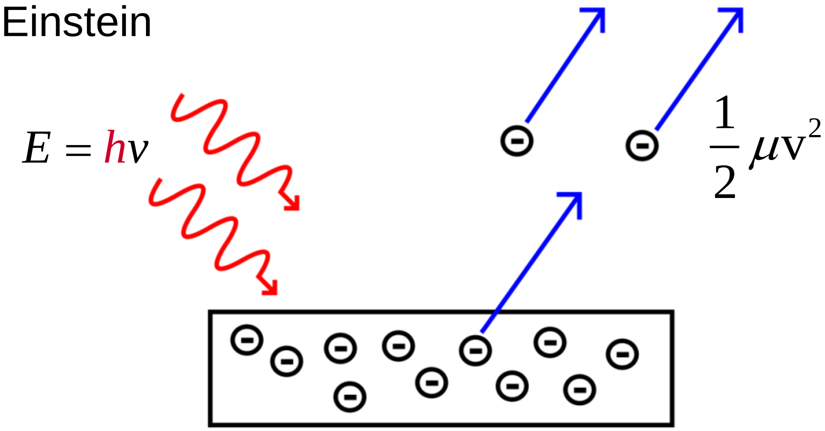
Max Planck, Albert Einstein,
Niels Bohr, Louis de Broglie

Max Born, Paul Dirac,
Werner Heisenberg, Wolfgang Pauli,
Erwin Schrödinger, Richard Feynman

Planck

$$E = nh\nu$$

Einstein



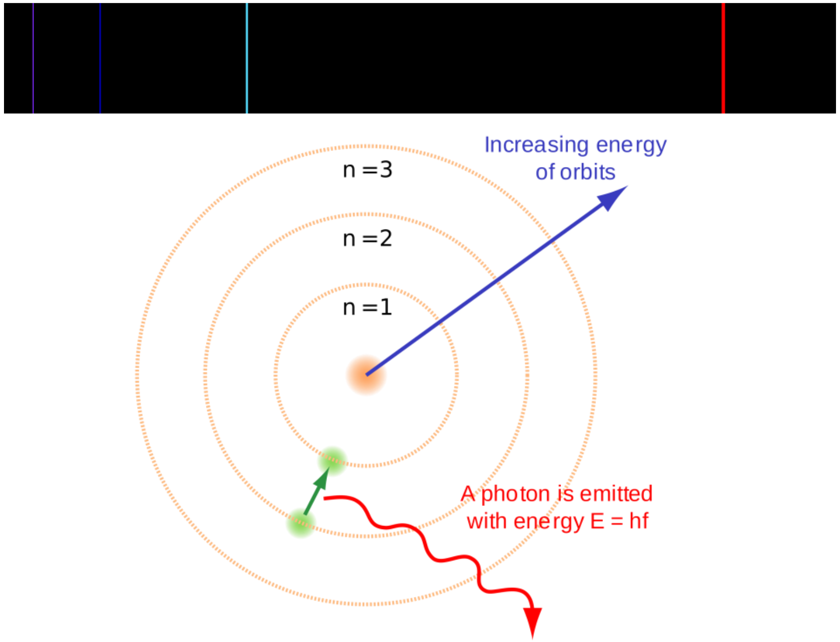
$$\frac{1}{2}\mu v^2 = h\nu - W_0$$

$$E = h\nu = \hbar\omega$$

$$E^2 = \mu_0^2 c^4 + c^2 p^2, E = cp$$

$$\mathbf{p} = \frac{E}{c}\mathbf{n} = \frac{h\nu}{c}\mathbf{n} = \frac{h}{\lambda}\mathbf{n} = \hbar\mathbf{k}$$

Bohr



de Broglie

Matter wave $E = h\nu = \hbar\omega \qquad \mathbf{p} = \frac{h}{\lambda}\mathbf{n} = \hbar\mathbf{k}$

$$E_k = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m} \qquad \vec{k} = \frac{2\pi}{\lambda}\vec{n}$$

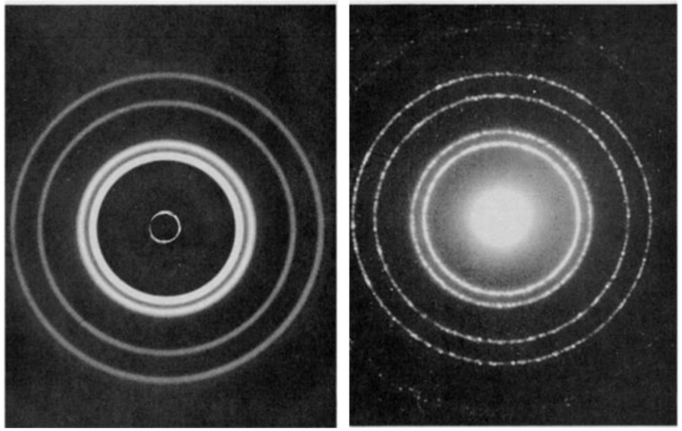
$\lambda_{\text{bullet of 10g,400m/s}} = 1.66 \times 10^{-34}\text{m} = 1.66 \times 10^{-24}\text{Å}$

$\lambda_{\text{electron of 100eV}} = 1.23 \times 10^{-10}\text{m} = 1.23\text{Å}$

A. Piccard, E. Henriot, P. Ehrenfest, E. Herzen, Th. De Donder, E. Schrödinger, J.E. Verschaffelt, W. Pauli, W. Heisenberg, R.H. Fowler, L. Brillouin;
B. P. Debye, M. Knudsen, W.L. Bragg, H.A. Kramers, P.A.M. Dirac, A.H. Compton, **L. de Broglie**, M. Born, N. Bohr;
I. Langmuir, M. Planck, M. Skłodowska-Curie, H.A. Lorentz, A. Einstein, P. Langevin, Ch. E. Guye, C.T.R. Wilson, O.W. Richardson

de Broglie's Hypothesis

1924 doctoral dissertation



1927

Prince Louis-Victor
de Broglie
(1892 – 1987)

The motion of a particle is governed by the wave propagation properties of matter wave

$$E_k = \frac{(\hbar k)^2}{2m}$$

Wave function ?

Chapter 1 Formation of Crystal

Wave function of free particle

$$\Psi(\mathbf{r},t)$$

$$E = h\nu = \hbar\omega \qquad \mathbf{p} = \frac{h}{\lambda}\mathbf{n} = \hbar\mathbf{k}$$

$$u(x,t) = A\cos(kx-\omega t)$$

$$\tilde{u}(x,t) = Ae^{\mathrm{i}(kx-\omega t)}$$

$$\Psi(x,t) = Ae^{\mathrm{i}(kx-\omega t)} = Ae^{-\frac{i}{\hbar}(Et-px)}$$

$$\Psi(r,t) = Ae^{-\frac{i}{\hbar}(Et-p_x x-p_y y-p_z z)} = Ae^{-\frac{i}{\hbar}(Et-\mathbf{p}\cdot r)}$$

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + U\Psi$$

Schrodinger Equation

$$\left|\Psi(\mathbf{r},t)\right|^2 = \Psi(\mathbf{r},t)\cdot\Psi^*(\mathbf{r},t)$$

probability density

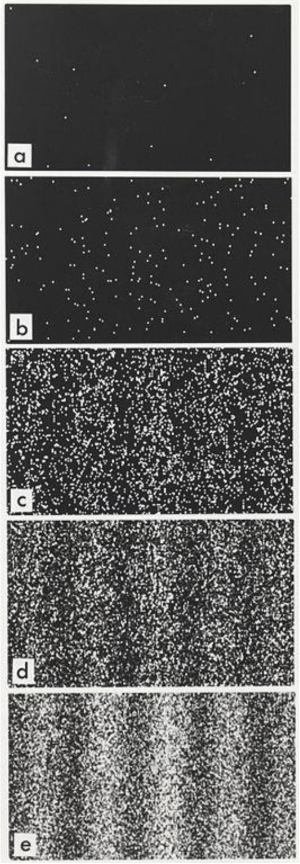
$$\mathrm{d}W(\mathbf{r},t) = C\left|\Psi\right|^2 \mathrm{d}x\mathrm{d}y\mathrm{d}z = C\left|\Psi\right|^2 \mathrm{d}\tau$$

$$W(\mathbf{r},t) = \int_V C\left|\Psi\right|^2 \mathrm{d}\tau$$

$$V \to \infty$$

$$\int_\infty C\left|\Psi\right|^2 \mathrm{d}\tau = 1$$

$$C = \frac{1}{\int_\infty \left|\Psi\right|^2 \mathrm{d}\tau}$$



A double slit experiment showing the accumulation of electrons on a screen as time passes.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + U\Psi$$

vs

$$\mathbf{F} = m\mathbf{a}$$

Schrodinger Equation of free particle

F=ma

$$\Psi = A\exp\left[-\frac{i}{\hbar}(Et-\mathbf{p}\cdot r)\right]$$

$$\Psi = A\exp\left[-\frac{i}{\hbar}(Et-(p_x\cdot x+p_y\cdot y+p_z\cdot z))\right]$$

$$\frac{\partial\Psi}{\partial t} = \left(-\frac{i}{\hbar}E\right)A\exp\left[-\frac{i}{\hbar}(Et-\mathbf{p}\cdot r)\right] = -\frac{i}{\hbar}E\Psi \qquad \textbf{(1)}$$

$$\frac{\partial^2\Psi}{\partial x^2} = -\frac{p_x^2}{\hbar^2}\Psi \qquad \frac{\partial^2\Psi}{\partial y^2} = -\frac{p_y^2}{\hbar^2}\Psi \qquad \frac{\partial^2\Psi}{\partial z^2} = -\frac{p_z^2}{\hbar^2}\Psi$$

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2} = -\left(\frac{p_x^2+p_y^2+p_z^2}{\hbar^2}\right)\Psi = -\frac{p^2}{\hbar^2}\Psi$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2} = \nabla^2\Psi = -\frac{p^2}{\hbar^2}\Psi$$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi = -\frac{\hbar^2}{2m}\cdot-\frac{p^2}{\hbar^2}\Psi = \frac{p^2}{2m}\Psi = E\Psi \qquad \textbf{(2)}$$

Combining eq. (1) and (2),

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi \qquad \textbf{(3)}$$

According to eq. (1),

$$E\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

According to eq. (2),

$$\nabla^2\Psi = -\frac{p^2}{\hbar^2}\Psi$$

$$(\mathbf{p}\cdot\mathbf{p})\Psi = \left[(-i\hbar\nabla)\cdot(-i\hbar\nabla)\right]\Psi$$

$$\mathbf{p}\Psi = -i\hbar\nabla\Psi$$

$$\nabla = \mathbf{i}\frac{\partial}{\partial x}+\mathbf{j}\frac{\partial}{\partial y}+\mathbf{k}\frac{\partial}{\partial z}$$

$$E \rightarrow i\hbar\frac{\partial}{\partial t}$$

$$\mathbf{p} \rightarrow -i\hbar\nabla$$

Schrodinger Equation of particle in a force field

Schrodinger Equation of free particle

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi \qquad \textbf{(3)}$$

$$E \rightarrow i\hbar\frac{\partial}{\partial t} \qquad \mathbf{p} \rightarrow -i\hbar\nabla$$

In a force field

$$U(\mathbf{r},t)$$

$$E = \frac{p^2}{2m} + U$$

$$E\Psi = \left(\frac{p^2}{2m} + U\right)\Psi$$

$$i\hbar\frac{\partial}{\partial t}\Psi = \frac{(-i\hbar\nabla)^2}{2m}\Psi + U\Psi$$

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + U\Psi \qquad \textbf{(4)} \longrightarrow \Psi(\mathbf{r},t)$$

Time-Independent Schrodinger Equation

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\Psi+U\Psi \qquad \textbf{(4)}$$

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t)+U(\mathbf{r},t)\Psi(\mathbf{r},t)$$

$U(\mathbf{r},t)\to U(\mathbf{r})$

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\Psi+U(\mathbf{r})\Psi$$

Separation of variables: $\Psi(\mathbf{r},t)=\psi(\mathbf{r})f(t)$

$$i\hbar\frac{\mathrm{d}f(t)}{\mathrm{d}t}\psi(\mathbf{r})=-f(t)\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+U(\mathbf{r})\psi(\mathbf{r})f(t)$$

$$\frac{i\hbar}{f(t)}\frac{\mathrm{d}f(t)}{\mathrm{d}t}=\frac{1}{\psi(\mathbf{r})}\left[-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+U(\mathbf{r})\psi(\mathbf{r})\right]$$

$$\frac{i\hbar}{f(t)}\frac{\mathrm{d}f(t)}{\mathrm{d}t}=E \qquad \textbf{(5)}$$

$$\frac{1}{\psi(\mathbf{r})}\left[-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+U(\mathbf{r})\psi(\mathbf{r})\right]=E \qquad \textbf{(6)}$$

According to eq. (5),

$$\frac{\mathrm{d}\ln f(t)}{\mathrm{d}t}=-iE/\hbar \qquad f(t)=e^{-\frac{i}{\hbar}Et}$$

E ?

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r})e^{-\frac{i}{\hbar}Et}$$

$$=i\hbar\psi(\mathbf{r})(-iE/\hbar)e^{-\frac{i}{\hbar}Et}$$

$E\to i\hbar\frac{\partial}{\partial t}$ $\qquad =E\psi(\mathbf{r})f(t)=E\Psi(\mathbf{r},t)$

According to eq. (6),

$$\left(-\frac{\hbar^2}{2m}\nabla^2+U\right)\psi=E\psi \qquad \textbf{(7)}$$

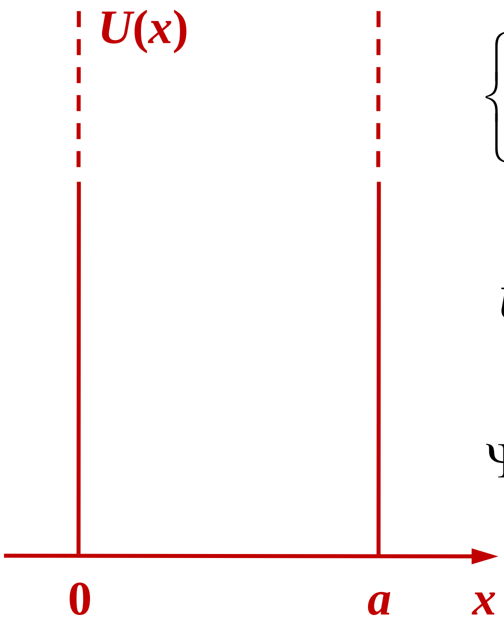
$$\hat{H}=-\frac{\hbar^2}{2m}\nabla^2+U$$

Eq. (7) ⟶ $\hat{H}\psi=E\psi$ **(8)**

Eq. (4) ⟶ $\hat{H}\Psi=i\hbar\frac{\partial}{\partial t}\Psi$ **(9)**

Infinite Potential Well

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



$$\begin{cases} U(x)=0, & 0<x<a \\ U(x)=\infty, & x>a, x<0 \end{cases}$$

$$U(x,t)\text{——}U(x)$$

$$\Psi(x,t)=\psi(x)\mathrm{e}^{-\mathrm{i}Et/\hbar}$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}=E\psi$$

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+\frac{2mE}{\hbar^2}\psi=0$$

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

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+k^2\psi=0$$

$$\psi=A\sin kx+B\cos kx$$

$$E=\frac{(\hbar k)^2}{2m}$$

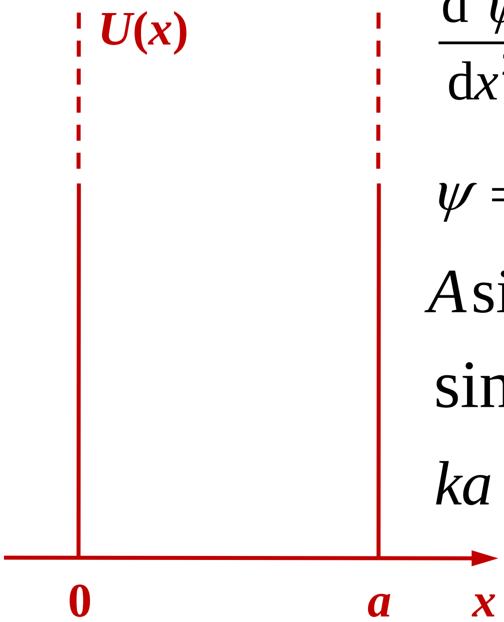
$$\psi(x)=0,\quad x>a, x<0$$

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

$$\psi(a)=A\sin ka+B\cos ka=0$$

$$B=0$$

$$A\sin ka=0$$



$$\frac{d^2\psi}{dx^2}+\frac{2mE}{\hbar^2}\psi=0 \qquad k=\frac{\sqrt{2mE}}{\hbar}$$

$$\psi = A\sin kx + B\cos kx$$

$$A\sin ka = 0$$

$$\sin ka = 0$$

$$ka = n\pi \qquad k = n\frac{\pi}{a}$$

$$n = 1, 2, 3, \ldots$$

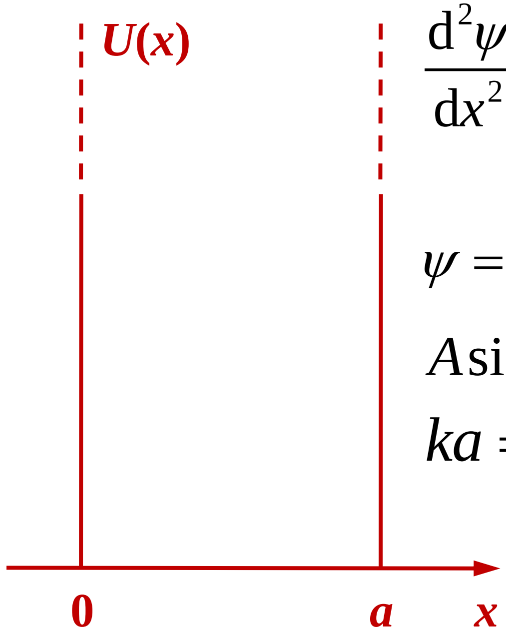
$$\psi(x) = A\sin\frac{n\pi}{a}x \qquad 0 \le x \le a$$

$$\int_0^a |\psi|^2 dx = 1 \qquad A=\sqrt{\frac{2}{a}}$$

$$\psi(x)=\sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x$$

$$|\psi_n|^2 = \frac{2}{a}\sin^2\frac{n\pi}{a}x$$

$$n = 1, 2, 3, \ldots$$



$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

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

$$\psi = A\sin kx + B\cos kx$$

$$A\sin ka = 0$$

$$ka = n\pi \qquad n = 1, 2, 3, \ldots$$

$$k = n\frac{\pi}{a}$$

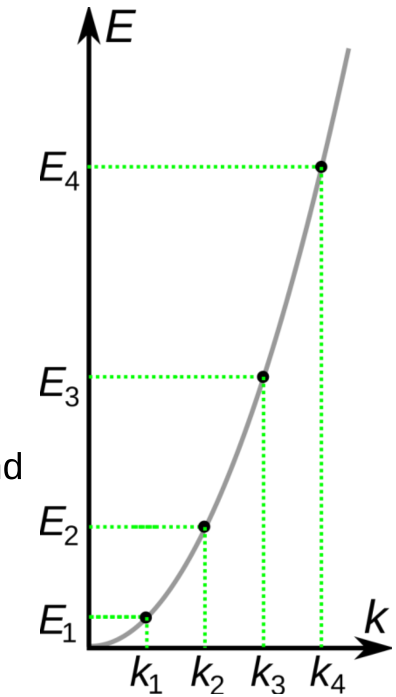
$$E = \frac{(\hbar k)^2}{2m}$$

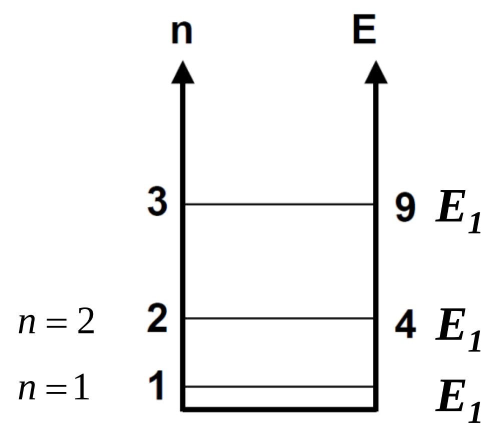
$$E = E_n = \frac{\pi^2\hbar^2}{2ma^2}n^2$$

$$n = 1, 2, 3, \ldots$$

$m\downarrow$, $a\downarrow$, $\Delta E\uparrow$, quantum effect strengthen → nano-material

The energy of a particle in a box (black circles) and a free particle (grey line) both depend upon wavenumber.





$$E_2 = \frac{2\pi^2\hbar^2}{ma^2}$$

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

Harmonic Oscillator

$$E = nh\nu\,?$$

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

$$\xi=\sqrt{\frac{m\omega}{\hbar}}x \qquad \lambda=\frac{2E}{\hbar\omega}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\psi(\xi)+(\lambda-\xi^2)\psi(\xi)=0$$

$$\lambda \ll \xi^2$$

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\psi-\xi^2\psi=0$$

$$\psi=e^{\pm\frac{1}{2}\xi^2} \longrightarrow \psi=e^{-\frac{1}{2}\xi^2}$$

Only this solution is accepted

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}e^{-\frac{1}{2}\xi^2}+(\lambda-\xi^2)e^{-\frac{1}{2}\xi^2}=-(1-\xi^2)e^{-\frac{1}{2}\xi^2}+(\lambda-\xi^2)e^{-\frac{1}{2}\xi^2}=0$$

$$\lambda=1 \qquad \psi_0=e^{-\frac{1}{2}\xi^2} \qquad E=\frac{1}{2}\lambda\hbar\omega=\frac{1}{2}\hbar\omega$$

$$\left(\psi_0''\right)'+\left[(1-\xi^2)\psi_0\right]'\equiv 0$$

$$\downarrow \quad \psi_0'=-\xi e^{-\frac{1}{2}\xi^2}=-\xi\psi_0$$

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\psi_0'+(3-\xi^2)\psi_0'\equiv 0$$

$$\lambda=3 \qquad \psi_1=\psi_0'=-\xi e^{-\frac{1}{2}\xi^2}$$

$$E=\frac{1}{2}\lambda\hbar\omega=\frac{3}{2}\hbar\omega$$

$$\lambda=5 \qquad \psi_2=(2\xi^2-1)e^{-\frac{1}{2}\xi^2}$$

$$E_n=\left(n+\frac{1}{2}\right)\hbar\omega \qquad (n=0,1,2,\cdots)$$

Harmonic Oscillator

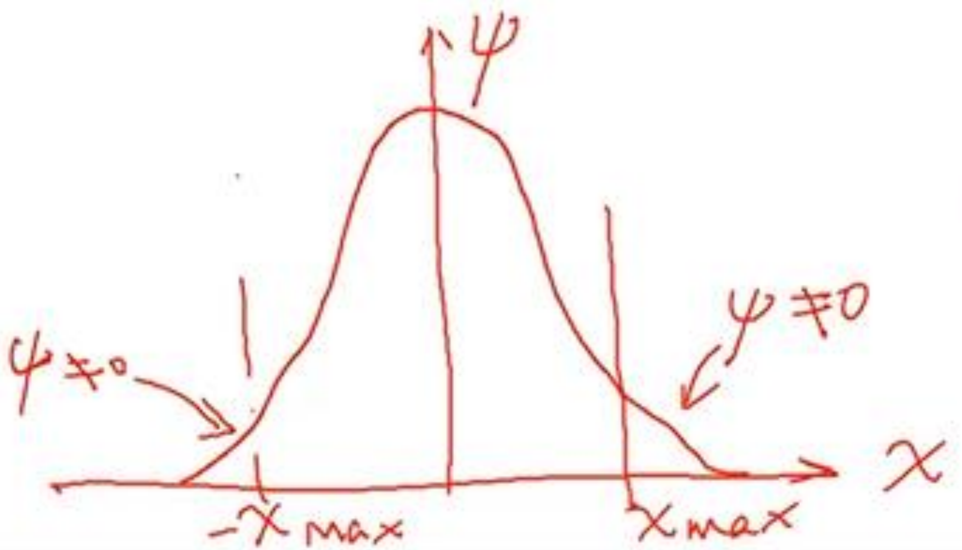
$$E = nh\nu\,?$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega = \left(n + \frac{1}{2}\right)h\nu$$

(1) Difference between adjacent energy levels is a constant *hυ* (E=Δ*hυ*), which is consistent with Planck's blackbody theory and different from energy levels in atoms or infinite potential wells.

(2) E(min)=½*hυ* (≠0), which is different from Planck's blackbody theory (E=n*hυ*, Emin=0)

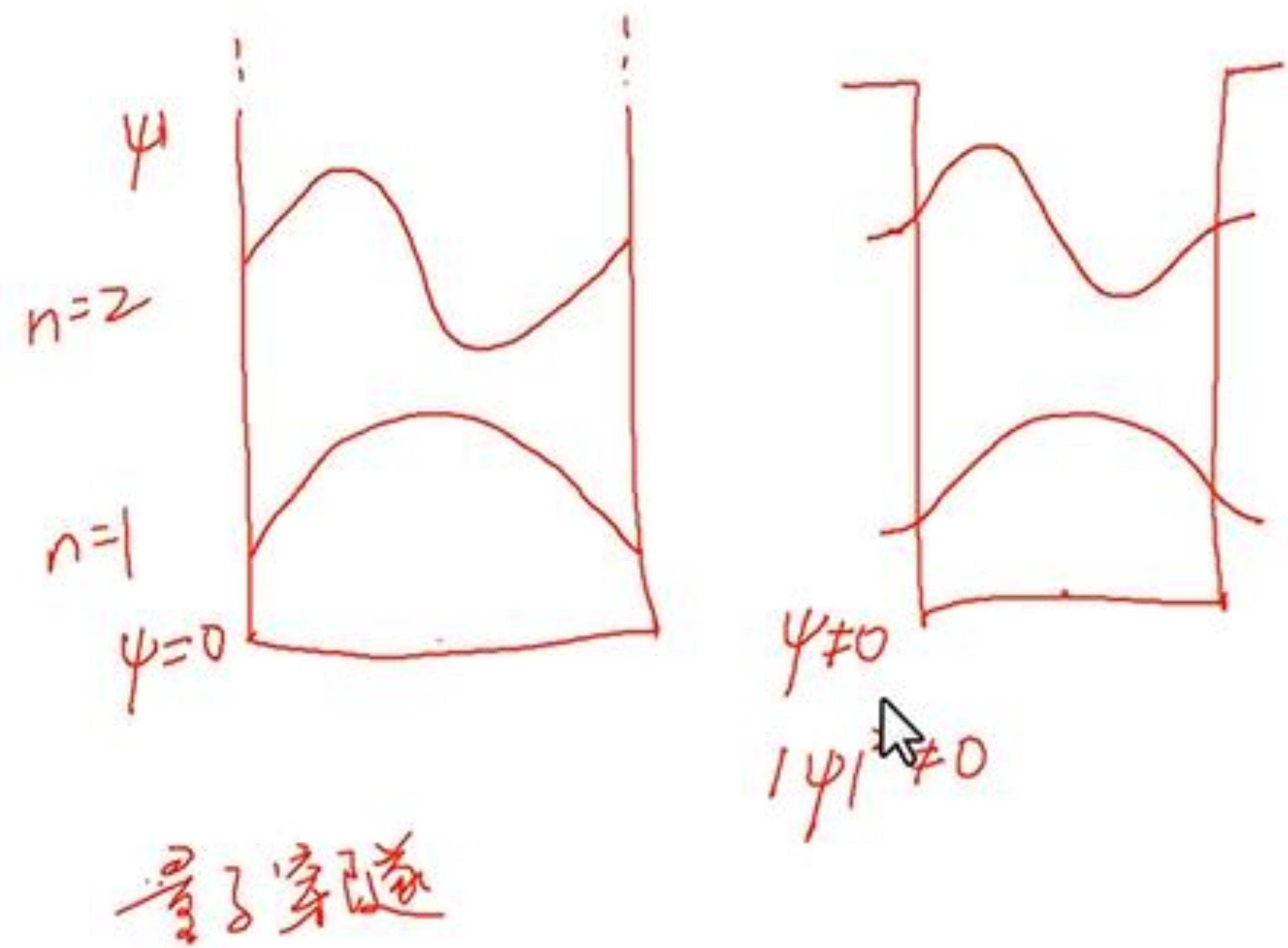
(3) In classical mechanics, the particle can not exceed *x*(max), but in quantum mechanics, the particle may exceed *x*(max) (with low probabilities)



Finite Potential Well

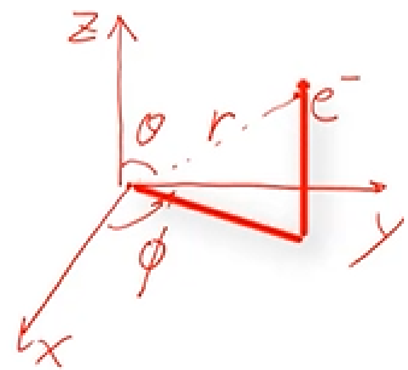
Quantum Tunneling

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



Atomic Structure   Schrodinger Equ. For H Atom

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



Schrodinger equ. becomes :

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

use separation of variables: $\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$

Schrodinger equ. becomes :

$$\frac{-\sin^2\theta}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{dR}}{\mathrm{d}r}\right)-\frac{2m}{\hbar^2}r^2\sin^2\theta(E-U)-\frac{\sin\theta}{\Theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)=\frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2}$$

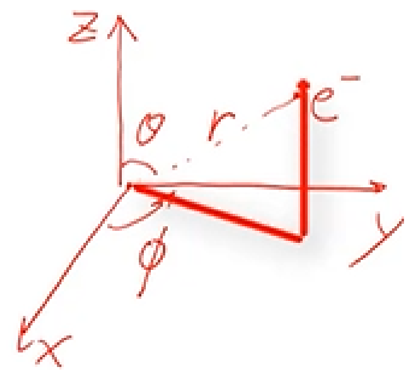
Both Equal to a constant

$$\begin{cases}\dfrac{1}{\Phi}\dfrac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2}=-m_l^2\\[2ex] \dfrac{1}{R}\dfrac{\mathrm{d}}{\mathrm{d}r}\left(r^2\dfrac{\mathrm{dR}}{\mathrm{d}r}\right)+\dfrac{2mr^2}{\hbar^2}(E-U)=\dfrac{m_l^2}{\sin^2\theta}-\dfrac{1}{\Theta}\dfrac{1}{\sin\theta}\dfrac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\dfrac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)\end{cases}$$

Both Equal to a constant

$$\begin{cases}\dfrac{1}{\Phi}\dfrac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2}=-m_l^2\\[2ex] \dfrac{m_l^2}{\sin^2\theta}-\dfrac{1}{\Theta}\dfrac{1}{\sin\theta}\dfrac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\dfrac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)=l(l+1)\\[2ex] \dfrac{1}{R}\dfrac{\mathrm{d}}{\mathrm{d}r}\left(r^2\dfrac{\mathrm{dR}}{\mathrm{d}r}\right)+\dfrac{2m}{\hbar^2}r^2(E-U)=l(l+1)\end{cases}$$

Atomic Structure Schrodinger Equ. For H Atom



$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\psi}{\partial r})+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\psi}{\partial\theta})+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2m}{\hbar}(E-U)\psi=0$$

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

$\Phi,\Theta,$R must be well-behaved functions

1. Ψ and dΨ/dx must be finite
2. Ψ and dΨ/dx must be single-valued
3. Ψ and dΨ/dx must be continuous

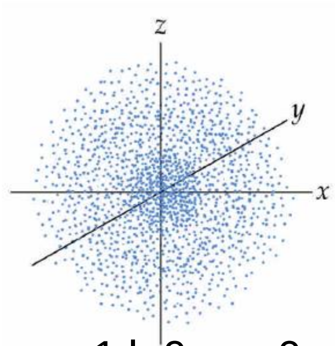
(1) Φ must be single-valued: $\mathrm{m_l} = 0, \pm1, \pm2, \ldots$

(2) Θ must be finite: $\mathrm{l} = 0, 1, 2, \ldots$ and $\mathrm{l} \geq |\mathrm{m_l}|$

(3) R must be finite: $E=E_n=-\frac{Z^2\mathrm{e}^4 m}{8\varepsilon_0^2\mathrm{h}^2}\frac{1}{n^2}$, n = 1, 2, 3, … and l < n

$$\begin{cases} n\text{: principle quantum number} \rightarrow \text{decide } \mathrm{E_n} \\ l\text{: orbital quantum number} \rightarrow 0,1,2,\ldots,n-1 \\ m_l\text{: magnetic quantum number} \rightarrow 0,\pm1,\pm2,\pm3,\ldots,\pm l \end{cases}$$

Features of the Atomic Wavefunctions



$n=1, l=0, m_l=0$

1s

完备的

一组量子数 (n, l, m_l, m_s)

$\updownarrow$

一个波函数 ψ

$\updownarrow$ $|\psi|^2$

一个量子态

$(1, 0, 0, \pm \frac{1}{2})$

$\updownarrow$

ψ

$\updownarrow$

量子态/轨道 $|\psi|^2$

Pauli's Exclusion Principle $\Rightarrow$ **no 2 electrons in a system (an atom or a solid) can be in the same quantum state (have the same n, l, m_l, m_s)**

Chapter 1 Formation of Crystal

1.1 Quantum Mechanics and atomic structure

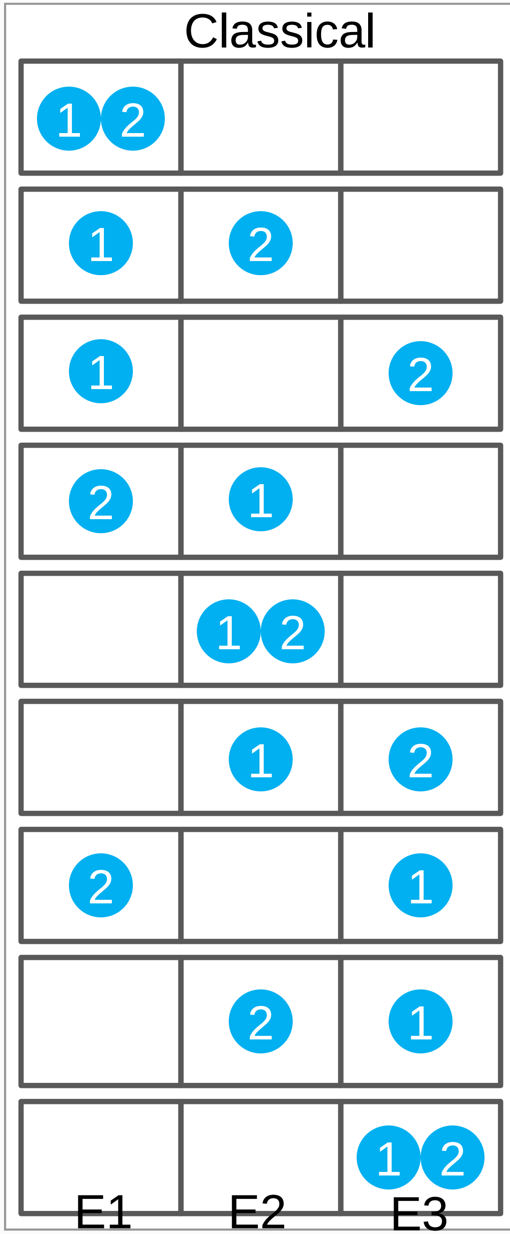
- 1.1.1 Electrons
- 1.1.2 Old quantum theory
- 1.1.3 Method of Quantum Mechanics
- 1.1.4 Distributing functions of micro-particles

1.2 Binding

1.3 Crystal structure and typical crystals

1.4 Reciprocal Lattice and Brillouin Zone

1.5 Defects in Solids



A system with N identical micro-particles, without either generation of new particles or vanishing of existed particles, without energy exchange
—an isolated system

Energy class:

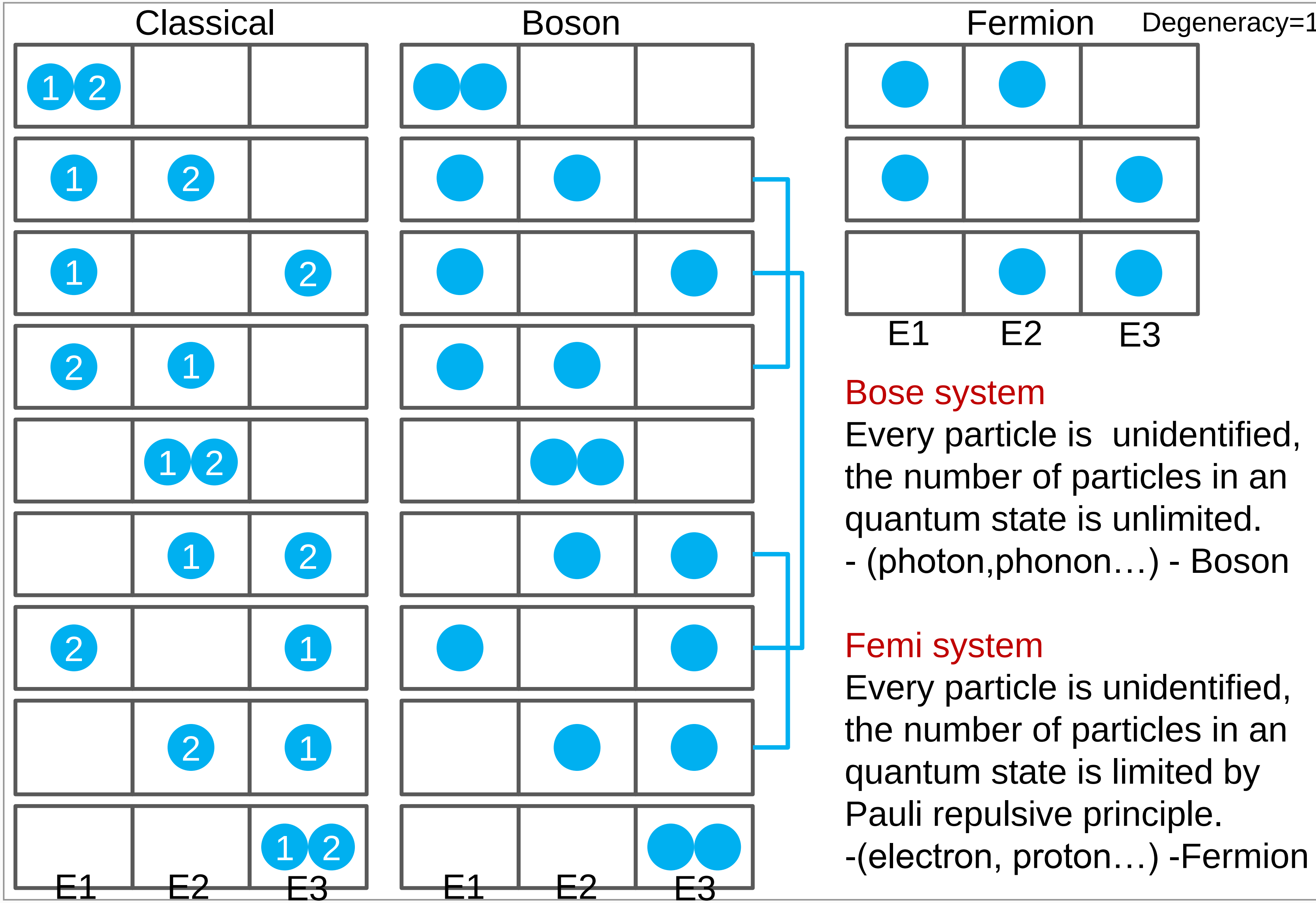
$E_1, E_2, E_3, \ldots, E_l, \ldots$

Particle number:

$a_1, a_2, a_3, \ldots, a_l, \ldots$

Boltzman system

Every particle is identified, the number of particles in an quantum state is unlimited.



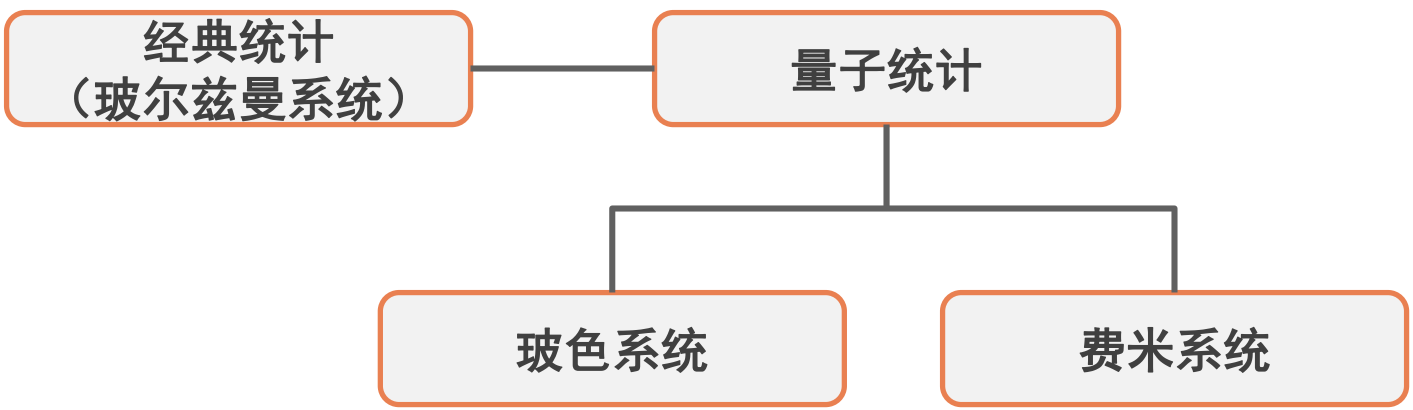
Bose system

Every particle is unidentified, the number of particles in an quantum state is unlimited.
- (photon,phonon…) - Boson

Femi system

Every particle is unidentified, the number of particles in an quantum state is limited by Pauli repulsive principle.
-(electron, proton…) -Fermion

全同性原理给量子统计和经典统计带来重要差别；
泡利不相容原理又给费米子和玻色子的统计带来重要差别。

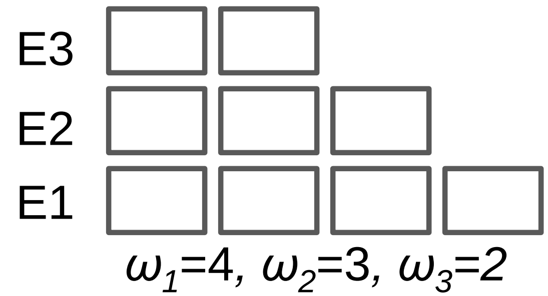


A system with volume *V* and energy *E* consists of many identical and independent particles. The total number of particles is *N*.

If
Energy level: $E_1, E_2, \ldots, E_l, \ldots$
Degeneracy: $\omega_1, \omega_2, \ldots, \omega_l \ldots$
Particle number: $a_1, a_2, \ldots, a_l \ldots$

$$\sum_l a_l = N$$

$$\sum_l a_l E_l = E$$



Boltzman system

$$a_l = \frac{\omega_l}{e^{\alpha+\beta E_l}}$$

Bose system

$$a_l = \frac{\omega_l}{e^{\alpha+\beta E_l} - 1}$$

Fermi system

$$a_l = \frac{\omega_l}{e^{\alpha+\beta E_l} + 1}$$

From statistical thermodynamics, the distribution function of particles in different systems can be gained as following:

Boltzman statistics

$$f_l = \frac{\alpha_l}{\omega_l} = \frac{1}{e^{(\alpha+\beta E_l)}} = \frac{1}{e^{(E_l-\mu)/k_BT}}$$

Bose-Einstein statistics

$$f_l = \frac{\alpha_l}{\omega_l} = \frac{1}{e^{(\alpha+\beta E_l)} - 1} = \frac{1}{e^{(E_l-\mu)/k_BT} - 1}$$

Fermi-Dirac statistics

$$f_l = \frac{\alpha_l}{\omega_l} = \frac{1}{e^{(\alpha+\beta E_l)} + 1} = \frac{1}{e^{(E_l-\mu)/k_BT} + 1}$$

$$\alpha = -\frac{\mu}{k_BT} \qquad \beta = \frac{1}{k_BT}$$

μ: chemical potential of a particle

Chapter 1 Formation of Crystal

· Summary

1 Basic Concept | **2 Train of Thought** | **3 Conclusions**

- Electron
- Old quantum theory
  - Blackbody radiation
  - Planck's theory
  - Einstein and Photon
  - Bohr and Atomic structure
  - de Broglie's Hypothesis
- Method of Quantum Mechanics
  - Wave function - Ψ
  - Schrodinger Equation
  - Expectation value
  - Properties of Ψ
  - Infinite Potential Well
  - Harmonic Oscillator
  - Quantum Tunneling
  - Atomic Structure
- Distributing functions
  - Quantum statistics
  - Fermi-Dirac distribution