

Summary

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1. The Atomic Nature

1.1 Electron and Charge

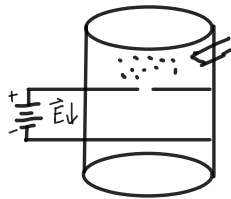
① Electrolysis (Faraday)

$m = \frac{QM}{FZ}$ there is charge inside atoms

② Discovery of electron (J.J. Thomson)

$d \left\{ \begin{array}{l} \frac{L}{FZ} \\ e^- \end{array} \right. \rightarrow \theta \quad \frac{e}{m} = \frac{v\theta}{B^2 L d} \text{ is a constant}$

③ Measurement of elementary charge (Millikan)



$$q_i = \frac{mg}{E} \frac{V_{r,i} + V_f}{V_f} \quad r = 3 \sqrt{\frac{9V_f}{2\rho g}}$$

ratio of q_i, q_j are rational numbers

$$V_f (w/o \vec{E}) \rightarrow r \rightarrow m \frac{V_r (w/ \vec{E})}{V_f} q_i$$

1.2 Atomic Models

① Rutherford's Model

High concentration of mass and charge at center (nucleus)

Small volume of nucleus compares to the whole atom

Orbiting electrons

② Bohr's Model

$$\frac{dE}{dL} = \omega \Rightarrow dL = \hbar \quad \text{Angular momentum is quantized}$$

$$r_n = \frac{n^2 \hbar^2}{m_e k e^2} \quad r_1 = \frac{\hbar^2}{m_e k e^2} = a_0 \quad \text{Bohr radius}$$

$$E_n = -\frac{k e^2}{2 a_0} \frac{Z^2}{n^2}$$

2. Particle Nature of Waves

2.1 Planck's Law

$$u(\lambda, T) \cdot d\lambda = \frac{\# \text{ of oscillators} \cdot \langle E \rangle}{\text{volume}} \quad \leftarrow \text{average energy of on oscillator}$$

$$\text{Energy is quantized: } E_n = nhf \quad P(E_n) = e^{-nhf/K_B T}$$

$$\langle E \rangle = \frac{\sum E_n P(E_n)}{\sum P(E_n)}$$

$$\# \text{ of oscillators: } \frac{4\pi k^2 dk}{(\pi/L)^3} \cdot \frac{1}{8} \cdot 2 \quad \leftarrow \begin{array}{l} k > 0 \\ 2 \text{ polarization} \end{array}$$

$$\therefore u(\lambda, T) = \frac{8\pi hc}{\lambda^5} \cdot \frac{1}{e^{hc/K_B T \lambda} - 1} \quad \left. \begin{array}{l} u(f, T) = \frac{8\pi h}{c^3} \cdot \frac{f^3}{e^{hf/K_B T} - 1} \end{array} \right\} \text{Planck's Law}$$

Small $\lambda \rightarrow$ Wien's Law

Large $\lambda \rightarrow$ Rayleigh-Jeans Law

2.2 Photoelectric Effect

$$K_{\max} = hf - \phi$$

$hf \sim$ Energy of photon as a particle

$\phi \sim$ Work function (need to free the electron)

2.3 Compton Scattering

Inelastic scattering \Rightarrow Particle Nature

$$\lambda' - \lambda = \Delta\lambda = \frac{h}{mc} (1 - \cos\theta)$$

$\frac{h}{mc} \sim$ Compton Wavelength Related to rest energy

2.4 Wave-Particle Duality: De Broglie Wave

$$\lambda = \frac{h}{p} = \frac{h}{mv} \sim \text{De Broglie Wavelength Related to momentum}$$

3. Wave Functions

3.1 Schrodinger Equation

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

Meaning: $|\psi(x,t)|^2 = \psi^*(x,t) \psi(x,t)$ is the probability density function of finding the particle at (x,t)

3.2 Operators

Operators are applied on wave functions to get specific physical quantities

$\hat{Q} \psi(x,t) = q \psi(x,t)$, q is the eigenvalue and $\psi(x,t)$ is the eigenstate

• Some operators

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad \hat{x} = x, \quad \hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V$$

• Expectation value of operators

$$\langle \hat{Q} \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{Q} \psi(x) dx$$

$i\hbar \frac{d}{dt} \langle \hat{Q} \rangle = \langle [\hat{Q}, \hat{H}] \rangle \Rightarrow$ if \hat{Q} and \hat{H} commutes [i.e. $[\hat{Q}, \hat{H}] = 0$], its expectation value would be a constant

3.3 Time-independent Schrodinger Equation

Assumption: V is only a function of $x \Rightarrow$ We could separate variables

Result: $\psi(x,t) = \psi(x) e^{-iEt/\hbar}$

Equation: $\hat{H} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V(x) \psi = E \psi$ E is the energy of particle

3.3.1 Stationary States

Quantum states with all observables independent of t .

Example. Probability density

$$\begin{aligned} & \int_{-\infty}^{\infty} \psi^*(x,t) \psi(x,t) dx \\ &= \int_{-\infty}^{\infty} \psi^*(x) e^{iEt/\hbar} \psi(x) e^{-iEt/\hbar} dx \\ &= \int_{-\infty}^{\infty} |\psi(x)|^2 dx \quad \text{is independent of time} \end{aligned}$$

3.3.2 Wave Packets

$\psi(x) = A e^{ikx} + B e^{-ikx}$ violates the uncertainty principle, thus $\psi(x)$ is a superposition of eigenstates $\psi_n(x)$ with different "weight" C_n .

$$\psi(x) = \sum_{n=1}^{\infty} C_n \psi_n(x) \quad \text{where} \quad C_n = \int_{-\infty}^{\infty} \psi_n^*(x) \psi(x, 0) dx$$

$|C_n|^2$ is the probability of returning E_n in a measurement, $\sum_{n=1}^{\infty} |C_n|^2 = 1$

Add the time-dependence:

$$\psi(x,t) = \sum_{n=1}^{\infty} C_n \psi_n(x) e^{-iE_n t/\hbar} = \sum_{n=1}^{\infty} C_n \psi_n(x,t)$$

Phase Velocity: Velocity of the carrier wave $v_p = \frac{\omega}{k} |_{k=k_0}$

Group Velocity: Velocity of the wave packet $v_g = \frac{d\omega}{dk} |_{k=k_0}$

3.3.3 General Procedure of solving a problem

$$\textcircled{1} \frac{d^2\psi}{dx^2} = -\frac{2m(V_0 - E)}{\hbar^2} \psi$$

$\textcircled{2}$ Solve this 2nd order ODE, the solution is $\begin{cases} \text{oscillatory} & V_0 < E \\ \text{exponential} & V_0 > E \end{cases}$

$\textcircled{3}$ Determine the constants using boundary conditions ($\psi(x)$ is continuous, and $\frac{d\psi}{dx}$ is continuous as long as no delta potential)

$\textcircled{4}$ Determine the last constant by normalization of $\psi(x)$

3.3.4 Examples of potentials

$\textcircled{1}$ Square Well: $V(x) = 0$ inside the well

$$\text{Infinite: } \psi(x) = \begin{cases} A \cos kx + B \sin kx & K = \frac{\sqrt{2mE}}{\hbar} \\ 0 & \text{outside of the well} \end{cases}$$

$$\psi(0) = \psi(L) = 0 \Rightarrow KL = n\pi, K = \frac{n\pi}{L}$$

$$\therefore E_n = \frac{\hbar^2 K^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

Finite: Follows the same procedure, but $\psi(x)$ is not 0 outside the well

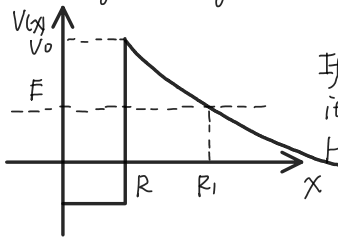
Penetration Depth: $\delta = \frac{1}{K} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$, when ψ decreased by $\frac{1}{e}$

$\textcircled{2}$ Harmonic Oscillator: $V(x) = \frac{1}{2}m\omega^2 x^2$

$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{m\omega x^2}{2\hbar}}$ is a Gaussian Distribution

$$E_0 = \frac{1}{2}\hbar\omega, E_n = (n + \frac{1}{2})\hbar\omega$$

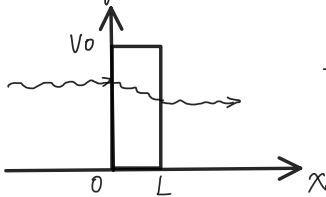
3.4 Tunneling: Ability to "Cross" the barrier



If the energy of particle, E , is less than V_0 , classically it's impossible to Cross the barrier.

However, in Quantum Mechanics, it happens.

3.4.1 Square Barrier



When the wave hits the barrier, both reflection and transmission happens. $T + R = 1$

$$T = \left[1 + \frac{V_0^2 \sinh^2(KL)}{4E(V_0 - E)}\right]^{-1} \text{ for bound states } E < V_0$$

if $E > V_0$, $K_2L = n\pi \Rightarrow T = 1$, full transmission since two reflection waves have a phase difference of π and cancels out.

3.4.2 Generalized Barrier

$$T = T_1 \cdot T_2 \cdot T_3 \dots \approx \exp\left(-\frac{2}{\hbar} \sqrt{2m} \int \sqrt{V(x) - E} dx\right)$$

Example. Alpha Decay

$$E = V(R_1) = \frac{2KZe^2}{R_1} \quad (Z \text{ is the atomic number of atom after decay})$$

$$T \approx \exp\left(-4\pi Z \sqrt{\frac{E_0}{E}} + 8\sqrt{\frac{R_1 Z}{r_0}}\right), \text{ where } r_0 = \frac{\hbar^2}{m_0 k e^2}, E_0 = \frac{K e^2}{2r_0}$$

3.4.3 Delta Potential: Discontinuity of $\frac{d\psi}{dx}$

$$V(x) = -S\delta(x)$$

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

$$\Rightarrow \frac{d\psi}{dx} \Big|_0^+ - \frac{d\psi}{dx} \Big|_0^- = -\frac{2mS}{\hbar^2} \psi(0) \text{ reveals discontinuity of } \frac{d\psi}{dx} \text{ at } x=0$$

4. Statistical Mechanics

4.1 Distribution of Particles

4.1.1 Discrete Distribution

There are different arrangements of N particles with total Energy E . Each arrangement corresponds to several microstates. Number of states corresponding to an energy level

is called degeneracy, g_i .

4.1.2 Continuous Distribution

$$n(E) dE = g(E) f(E) dE \quad \text{General Formula for all distributions}$$

$n(E)$: number of particles per volume between E and $E+dE$

$g(E)$: density of states

$f(E)$: probability that a particle occupies energy level E

4.2 Classical Statistics: Distinguishable Particles

4.2.1 Maxwell-Boltzmann Distribution

$$f_{MB}(E) = A e^{-E/k_B T}$$

$\therefore E = \frac{1}{2}mv^2$ for ideal gas

$$n(v) = \frac{4\pi N}{V} \left(\frac{m}{2\pi k_B T} \right)^{3/2} v^2 e^{-\frac{mv^2}{2k_B T}} = g(v) f_{MB}(v)$$

4.2.2 Velocities of ideal gas

① Most probable velocity

$$\frac{d}{dv} n(v) \big|_{v=v_{mp}} = 0$$

$$\therefore v_{mp} = \sqrt{\frac{2k_B T}{m}}$$

② Average velocity

$$\bar{v} = \frac{\int_0^\infty v n(v) dv}{\int_0^\infty n(v) dv} = \sqrt{\frac{8k_B T}{\pi m}}$$

③ Root-mean-square velocity

$$v_{rms} = \sqrt{\overline{v^2}} = \left(\frac{\int_0^\infty v^2 n(v) dv}{\int_0^\infty n(v) dv} \right)^{1/2} = \sqrt{\frac{3k_B T}{m}}$$

$$v_{rms} > \bar{v} > v_{mp}$$

4.2.3 Equipartition Theory

1 degree of freedom $\rightarrow \frac{1}{2}k_B T$ Energy

• Some examples

1D oscillators: $2 \cdot \frac{1}{2}k_B T = k_B T$

3D atoms: $3 \cdot \frac{1}{2}k_B T = \frac{3}{2}k_B T$

3D oscillators: $6 \cdot \frac{1}{2}k_B T = 3k_B T$

4.2.4 Validity of Classical Statistics

Maxwell-Boltzmann Distribution is valid when wave functions do not interact.

In other words, distance between adjacent particles, d , is greater than λ .

$$\Delta P_x = \sqrt{\overline{P_x^2} - \overline{P_x}^2} \quad \overline{P_x} = 0 \text{ because velocity has 2 directions}$$

$$\therefore \Delta P_x = \sqrt{\overline{P_x^2}} = \sqrt{mk_B T} \quad \Delta x \Delta P_x \geq \frac{\hbar}{2}$$

$$\therefore d = \left(\frac{V}{N} \right)^{1/3} \gg \frac{\hbar}{2\Delta P_x}$$

$$\therefore \frac{N}{V} \frac{\hbar^3}{8(mk_B T)^{3/2}} \ll 1$$

So, ① High concentration of particles, ② Low temperature and ③ small mass particle would violate classical distribution.

4.3 Quantum Statistics: Indistinguishable Particles

4.3.1 Bosons and Fermions

Bosons: Spins $(0, 1, 2, \dots)$, could have many in a state

Fermions: Spins $(\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots)$, obeys Pauli's Exclusion Principle, only 1 in a quantum state.

4.3.2 Bose-Einstein Distribution

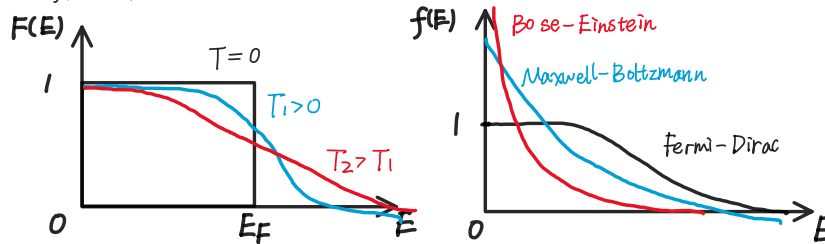
$$f_{BE} = \frac{1}{e^{(E-\mu)/k_B T} - 1} \quad \mu \text{ is the chemical potential}$$

4.3.3 Fermi-Dirac Distribution

$$f_{FD} = \frac{1}{e^{(E-\mu)/k_B T} + 1}$$

4.3.4 Fermi Energy

$\mu(T=0K) = E_F$ is Fermi Energy
 It's defined as the energy difference between highest and lowest occupied single-particle states of non-interacting Fermions at $T=0K$.
 $\therefore f_{FD}(E_F) = \frac{1}{2}$



4.4 Applications of Quantum Statistics

Bose-Einstein Distribution:

4.4.1 Blackbody Radiation

$$u(E) dE = E n(E) dE = E g(E) f_{BE}(E) dE$$

$$= \frac{8\pi E^3}{(hc)^3 (e^{E/k_B T} - 1)} dE$$

Substitute $E = hf$, $dE = h df$

$$u(f, T) = \frac{8\pi h f^3}{c^3 (e^{hf/k_B T} - 1)} \quad \text{Planck's Law}$$

4.4.2 Specific Heat of Solid

Atoms as Quantum Harmonic Oscillators

$$U = 3NA \bar{E} = \frac{3NA \hbar \omega}{e^{\hbar \omega / k_B T} - 1}$$

$$C_V = \frac{\partial U}{\partial T} = 3R \left(\frac{\theta_E}{T} \right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2}, \quad \theta_E = \frac{\hbar \omega}{k_B} \text{ is Einstein temperature}$$

① High temperature: $e^{\theta_E/T} \approx 1 + \frac{\theta_E}{T}$ $C_V \approx 3R$ like classical theories

② Low temperature: $C_V \approx 3R \left(\frac{\theta_E}{T} \right)^2 e^{-\theta_E/T}$

Fermi-Dirac Distribution:

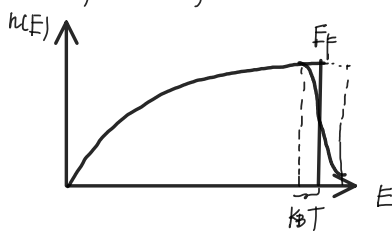
4.4.3 Free Electron Gas Model of Metals

Problem: C_V of metal $< \frac{9}{2}R$ predicted, due to the electron's part ($\frac{3}{2}R$)

$$n(E) = g(E) f_{FD}(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E} \cdot \frac{1}{e^{(E-E_F)/k_B T} + 1}$$

fraction of electron available: Fermi Sea

should use $n(E)$, but at low temperature approximately same



$$\frac{k_B T g(E_F)}{\int_0^\infty g(E) dE} = \frac{k_B T \sqrt{E_F}}{\int_0^{E_F} \sqrt{E} dE} = \frac{\frac{3}{2} k_B T}{E_F} = \frac{3}{2} \frac{T}{T_F}$$

where $T_F = \frac{E_F}{k_B}$ is Fermi Temperature

$\frac{T}{T_F} \approx \frac{1}{200}$, so specific heat of electron is much less than predicted. ($\frac{3}{2}R$)