Lecture 1 Early stage of quantum physics

Monday, April 29, 2024

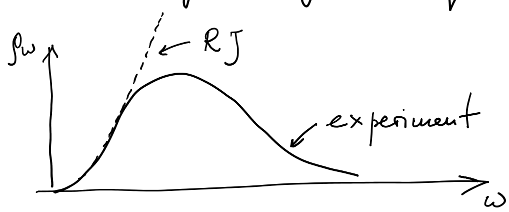
## 1.1 thermal e/m radiation and ultraviolet catastrophy

End of XIX century

- All bodies with $T \neq 0$ are sources of e/m radiation
- Thermal radiation: the body is in thermal equilibrium with all surrounding bodies $\Rightarrow$ determined by $T$
- Black body (black body cavity): ideal absorber/emitter of thermal radiation (no radiation passing through or being reflected)
- Experiments on black body radiation

$\to$ energy density $u = \frac{U}{V} = \int_0^\infty \rho_\omega \, d\omega$

$\rho_\omega$ – spectral density of e/m radiation




$\to$ exper: $u = \alpha T^4$ [Stefan–Boltzmann]

$\to$ exper: $\omega_{max} \propto T$ [Wien's displacement]

- Classical theory of e/m radiation

$$\rho_\omega = \frac{\omega^2}{\pi^2 c^3} k_B T \quad \text{[Rayleigh–Jeans]}$$

$u = \infty$ ??? Ultraviolet catastrophy

## 1.2 Planck hypothesis and Planck constant

Nov 1900 Planck RJ $\Longrightarrow$ $\rho_\omega = \underbrace{\frac{\omega^2}{\pi^2 c^3}}_{\text{number of oscillators in RJ theory}} \langle E \rangle$

$\langle E \rangle$ – mean energy of oscillator/standing e/m wave in cavity

Planck's revolutionary hypothesis: energy of oscillator changes with discrete quanta of energy $\hbar\omega$. $\hbar = \frac{h}{2\pi}$ Planck constant

$$\langle E \rangle = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1} = \frac{1}{2}\hbar\omega \coth\frac{\hbar\omega}{2k_B T}$$

quantum Gibbs

Modern result

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

$\rho_\omega = \rho_\omega^{(0)} + \rho_\omega^T$, forget about $\rho_\omega^{(0)}$

$$\boxed{\rho_\omega^T = \frac{\omega^2}{\pi^2 c^3} \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}}$$

[Planck formula]

Remark 1. Angular frequency $\omega = 2\pi\nu$

$$\rho_\omega d\omega = \rho_\nu d\nu \Rightarrow \rho_\nu = \rho_{\omega\to\nu}\frac{d\omega}{d\nu} = \frac{8\pi h\nu^3}{c^3}\frac{1}{e^{h\nu/k_BT}-1}$$

Remark 2. At $\frac{\hbar\omega}{k_BT} \ll 1 \Rightarrow$ Planck $\to$ RJ

Remark 3. $u = \int_0^\infty \rho_\omega^T d\omega = \alpha T^4$ [S-B] exp. value $\alpha \Rightarrow$ value of $\hbar$

## (1.3) Concept of photon

(a) photoelectric effect: emission of electrons from metal surface caused by light — major puzzle in physics in early 1900s

Experimental laws of phot. effect:

1) number of electrons emitted per unit time $\propto$ light intensity;
2) kinetic energy of emitted electrons does not on light intensity;
3) effect possible if $\omega > \omega_{cr}$
   kinetic energy of electrons $\propto \omega - \omega_{cr}$

E/m theory unable to explain 2) and 3)

Einstein 1905 with energy balance equation

$$\hbar\omega = A + \frac{mv^2}{2}$$

$\hbar\omega$ — energy of light quanta (photon)

$A$ — work function: energy required to remove electron from the surface

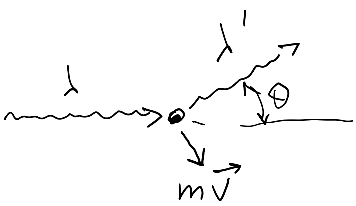
$\frac{mv^2}{2}$ — kinetic energy of electron

$$A = \hbar\omega_{cr} \Rightarrow \frac{mv^2}{2} = \hbar(\omega - \omega_{cr}) \quad \#3)$$

(b) Compton effect : interaction of X-rays (Röntgen rays, high-energy e/m radiation) with matter

Classical e/m theory (Thomson scattering)

Compton (1922-23): spectrum of scattered radiation $\lambda, \omega$ (incident radiation) AND $\underbrace{\lambda', \omega', \ \omega' < \omega, \ \lambda' > \lambda}_{\text{contradicts classical e/m theory}}$




$$\Delta\lambda = \lambda' - \lambda = 2\lambda_e \sin^2(\theta/2)$$

$\lambda_e \sim 2.4 \cdot 10^{-10}$ cm Compton constant

Explanation: Momentum of photon $\vec{p} = \hbar \vec{k}$

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

Two conservation laws

$$\left.\begin{aligned} \hbar\omega &= \hbar\omega' + \frac{m_e v^2}{2} \\ \hbar\vec{k} &= \hbar\vec{k}' + m_e\vec{v} \end{aligned}\right\} \quad \lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

Conclusion: E/m radiation behave like a wave (interference and diffraction experiments), but also have a particle nature (photoelectric and Compton effects)

(1.4) Nuclear model of atom

(a) Two basic models

- known at the begging of XX century:
  - existence of positive ions
  - electron
  - atom is complex electrical system $\sim 10^{-8}$ cm;
  - model ?

d

- Thomson's model (plum pudding model)
  Atoms are uniform spheres of positively charged matters in which electons are embedded;
- Planetary model:
  - Sun $\Leftrightarrow$ positive nucleus with $Ze$, $Z$ serial No of an element in periodic table
  - planets $\Leftrightarrow$ electrons.

(b) Rutherford experiments on scattering $\alpha$-particles (helium nuclei = 2 protons, 2 neutrons) $\Rightarrow$
$\Rightarrow$ planetary model

- upper bound of nucleus size
  $r \sim 10^{-13}$ cm $<<$ atom size $\sim 10^{-8}$ cm

- problem of planetary model:
  - angular velocity of electron
    $$m\omega^2 r = \frac{e^2}{r^2} \Rightarrow \omega = \sqrt{\frac{e^2}{mr^3}}$$
  - classical e/m theory: energy of electron $\to$
    $\to$ energy e/m radiation

$$\frac{dE}{dt} = -\underbrace{\gamma}_{\sim 10^8\ \text{sec}^{-1}} E \qquad \gamma = \frac{2e^2\omega^2}{3mc^3} \quad \text{radiation friction}$$

Conclusion: after $10^{-8}$ sec electron "falls down" on the nucleus $\Rightarrow$ atom is unstable system ???

## 1.5 Bohr theory

(a) Bohr's postulates

- Atom exists for a long time in certain stationary states with discrete spectrum of energies
  $E_1, E_2, \ldots$

- Transition from one stationary state with $E_n$ to another $E_m < E_n$ is accompanied by emission of light quanta

$$\hbar\omega_{mn} = E_m - E_n$$

(b) Quantization rules for circular orbits of electrons in atom

- Angular momentum $m_e v_e r = n\hbar$ (*)
  $n$ : principal quantum number, $n = 1, 2, 3$
- Radius of orbit from Newton law

$$\frac{mv^2}{r} = \frac{Ze^2}{r^2} \Rightarrow v^2 = \frac{Ze^2}{m_e r} \underset{\uparrow\,(*)}{=} \frac{n^2\hbar^2}{m_e^2 r^2} \Rightarrow$$

$$\Rightarrow \boxed{r = \frac{\hbar^2 n^2}{Z m_e e^2}} \quad (**)$$

- 1st Bohr orbit (of hydrogen atom), $n = 1$, $Z = 1$

$$r_0 \equiv a_0 = \frac{\hbar^2}{m_e e^2} \cong 0.5 \cdot 10^{-8}\ \text{cm}$$

- energy of electron in atom at $n$-th level

$$E_n = \underset{\substack{\parallel \\ \frac{m_e v^2}{2} \\ \parallel\,(*) \\ \frac{Ze^2}{2r}}}{E_{kin}} + \underset{\substack{\parallel \\ -\frac{Ze^2}{r}}}{E_{pot}} = -\frac{Ze^2}{2r} \underset{\uparrow\,(**)}{=} -\frac{Ze^2}{2}\frac{Z m_e e^2}{\hbar^2 n^2} \Rightarrow$$

$$\Rightarrow \boxed{E_n = -\frac{m_e Z^2 e^4}{2\hbar^2 n^2}} \quad (***)$$

$n = 1$
energy of ground state

Remarks 1) $\min E_n$ at $n=1$

2) $n \to \infty$ $E_n \to 0$

(c) Two more quantum numbers (Sommerfeld, Debye)

- q.n. $l$ : determines the shape of electron's orbital

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

- magnetic q.n. $m$ : orientation in space of partical orbital

  $m\hbar$ = component of atom's angular momentum along the magnetic field

  $-l \le m \le l$ , $2l+1$ values of $m$ $\Rightarrow$

$\Rightarrow$ number of allowed directions of angular momentum vector in magnetic field:

space quantization of angular momentum

(d) Summary of early amendments to Bohr theory

- Energy of electron in atom is determined by 3 q.n
- Transition from one energy state to another involves change of one or more q.n.
- In transition electron absorbs or emits lights of particular frequency

$$E_{final} - E_{initial} = \hbar\omega = h\nu$$

- However: atom is placed in magnetic field $\Rightarrow$

$\Rightarrow$ multiplicity of spectra (all the observed frequencies) cannot be explained by space quantization rules alone (with $n, l, m$)

Sommerfeld (1920): Another quantum number (inner q.n.)?

## 1.6 Birth of "spin".

- Kronig (1925): in addition to orbital angular momentum ⟹ angular momentum caused by spinning of electron about its own axis

  Kronig postulated ang mom $= \frac{\hbar}{2}$ (why?)

- Kronig able to explain the multiplicity of spectra, but: rotation rate is 130 times of $c = 3 \cdot 10^8$ m/sec ⟹

  ⟹ Kronig never published his idea

- Uhlenbeck & Goudsmit: the same spinning idea in Naturwissenschaften

- Kronig: letter in Nature criticizing U-G

- U-G: publish 2nd paper in Nature

  1st paper has a discrepancy of the factor of 2 with experimental result

- Thomas (1926): Factor of 2 correction

BUT

Q1. Why the spin angular momentum is quantized?

Q2. Why the idea cannot be reconciled with special theory of relativity?

# Chapter 2. Schrödinger Equation

## 2.1 DeBroglie waves. Wave properties of particles

- E/m radiation: first wave-like, then particle-like properties (corpuscular properties of light)

  Photon $E = \hbar\omega$, $p = \hbar\vec{k}$ (1)

- Matter: first particle-like then wave-like properties

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deBroglie hypothesis (1923): (1) are valid for particles with non-zero rest mass

Wave-like characteristics

$$\omega = \frac{E}{\hbar}, \quad \lambda_B = \frac{2\pi}{k} = \frac{2\pi\hbar}{p} = \frac{2\pi\hbar}{mv} = \frac{h}{mv} \quad (2)$$

$\lambda_B$ ↑ DeBroglie wavelength

$\Rightarrow$ wave field for particles characterized by wave function $\psi(\vec{r}, t)$

- probabilistic interpretation

$$|\psi(\vec{r}, t)|^2 \frac{d\vec{r}}{V} = \Pr\{\vec{r} \le \vec{r}(t) < \vec{r} + d\vec{r}\} \quad (3)$$

$$\int |\psi(\vec{r}, t)|^2 \frac{d\vec{r}}{V} = 1$$

- Monochromatic deBroglie wave ($E$ and $\vec{p}$ fixed)

Analogue of $e^{-i\omega t + i\vec{k}\vec{r}}$

$$\psi(\vec{r}, t) = C \exp\left(-\frac{iEt}{\hbar} + \frac{i\vec{p}\vec{r}}{\hbar}\right) \quad (4)$$

$$|\psi|^2 = \psi\psi^* = C^2$$

Remark. Normalization If (3) $\Rightarrow C = 1$

$$\text{If } \int |\psi(\vec{r}, t)|^2 d\vec{r} = 1 \Rightarrow C = \frac{1}{\sqrt{V}} \quad (5)$$

Remind Bohr quantization rule for angular momentum

$$\underbrace{m_e v}_{\frac{h}{\lambda_B}\ (2)} r_n = n\hbar \Rightarrow \boxed{2\pi r_n = n\lambda_B} \quad (6)$$

stationary orbits: integer number of deBroglie waves

Experiments fully confirm de Broglie hypothesis about wave properties of the particles with non-zero mass.

## 2.2 Wave equation for particles – Schrödinger eq

(a) Equation for free particle

$$E = \frac{p^2}{2m} \Rightarrow \boxed{\hbar\omega = \frac{\hbar k^2}{2m}} \quad (7)$$

example of quantum dispersion relation

$$\Downarrow$$

$$\boxed{i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi(\vec{r},t)} \quad (8)$$

Check $\psi(\vec{r},t) \sim \exp(-i\omega t + i\vec{k}\vec{r})$

(b) Momentum and Hamiltonian operators

$$\hat{H} = \hat{K} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\Delta_r$$

momentum operator $\hat{p} = -\frac{i}{\hbar}\frac{\partial}{\partial \vec{r}} = -\frac{i}{\hbar}\nabla_r$, from (8)

$$\boxed{i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \hat{H}\psi(\vec{r},t)} \quad (9)$$

- Next step: Eq. (9) is valid in general case

Example 1. Particle in potential field $U(\vec{r},t)$

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta_r + U(\vec{r},t) \equiv \frac{\hat{p}^2}{2m} + U(\vec{r},t)$$

Example 2. N-particle system

$$\hat{H} = \sum_{1\le i\le N}\left(-\frac{\hbar^2}{2m}\Delta_{r_i} + U(\vec{r}_i,t)\right) + \sum_{1\le i<j\le N}\Phi(|\vec{r}_i - \vec{r}_j|)$$

(c) Stationary solution

Go back to (9), sick solution for the time independent

$$\psi(\vec{r}, t) = \exp\left(-\frac{iEt}{\hbar}\right)\psi_E(\vec{r})$$

$$\hat{H}\psi_E(\vec{r}) = E\psi_E(\vec{r})$$

$$\Downarrow$$

$\psi_E(\vec{r})$ eigenfunction of Hamilton, $E$ eigenvalue

Dual role $\hat{H}$

1. $i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$ time evolution of the system considered

2. $\hat{H}\psi_E = E\psi_E$ energies and eigenfunctions of stationary states

Q. How to include spin in Schrödinger eq ?