Notes on Atomic Physics

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Conventions and Notation

Unit System Gaussian natural unit system with

$$c = \hbar = 1 \quad \text{and} \quad \varepsilon_0^{-1} = \mu_0 = 4\pi$$

Index System Einstein summation convention with

$$a_i b^i = \sum_i a_i b^i$$

Unit Conversion

Length $1\ \mathrm{eV}^{-1} \sim 197\ \mathrm{nm}$ **Mass** $1\ \mathrm{eV} \sim 1.78 \times 10^{-36}\ \mathrm{kg}$
Time $1\ \mathrm{eV}^{-1} \sim 6.58 \times 10^{-16}\ \mathrm{s}$
Electron Charge $e = \sqrt{\alpha} = 0.085$ **Fine Structure Constant** $\alpha = 1/137 \sim 0.0073$

Particle Properties of Waves

Electromagnetic Waves

The **speed of light** (electromagnetic waves):

$$c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$$

This equality is easily seen under Gaussian unit system.
Principle of Superposition → diffraction

Black Body Radiation

A **black body** is an idealized physical body that absorbs all incident electromagnetic radiation, regardless of frequency or angle of incidence.
Black-body radiation is the type of electromagnetic radiation within or surrounding a body in thermodynamic equilibrium with its environment, or emitted by a black body.

Rayleigh-Jeans Formula

$$u(\nu) = \bar{\varepsilon} G(\nu) = 8\pi kT\, \nu^2 \mathrm{d}\nu$$

Plank Formula

$$u(\nu) = 16\pi^2 \frac{\nu^3 \mathrm{d}\nu}{\exp\{\nu/2\pi kT\} - 1}$$

Actual Average Energy per Standing Wave

$$\bar{\varepsilon}_0 = \frac{2\pi\nu}{\exp\{\nu/2\pi kT\} - 1}$$

Photoelectric Effect

Photoelectric Effect

$$2\pi\nu = K + \phi$$

where $\phi = 2\pi\nu_0$ is the **work function**.

X-ray Diffraction

Braking Radiation: radiation generated by sudden acceleration of electron.
X-ray Production: $\lambda = 1.24 \times 10^{-6} \cdot V^{-1}$ where V is the voltage.

Bragg Diffraction $2d \sin\theta = n\lambda, \quad n \in \mathbb{Z}_+$

Compton Effect

Compton Wavelength $\lambda' - \lambda = \lambda_C (1 - \cos\phi)$
where target is usually electron with $\lambda_C = 2\pi/m_e \sim 2.426\ \mathrm{pm}$

Pair Production

Pair Production $e^+ + e^- \leftrightarrow \gamma + \gamma$

Photon Absorption

Photon Absorption $-I^{-1}\mathrm{d}I = \mu \mathrm{d}x$

Classical Gravitational Red Shift

Classical Gravitational Red Shift

$$\frac{\Delta\nu}{\nu} = \frac{GM}{R}$$

Wave Properties of Particles

De Broglie Waves

De Broglie Wavelength $\lambda = 2\pi/p$

Group Velocity and Phase Velocity

Wave Formula $A_\mu = C_\mu \cos(\omega t - k \cdot x)$
Phase Velocity $\phi = \omega t - k \cdot x = 0 \Rightarrow v_p = \omega \cdot k^{-1} = v^{-1}$
Group Velocity $\mathrm{d}\omega/\mathrm{d}k = 0 \Rightarrow v_g = v$

Particle Diffraction

Same as Bragg diffraction $2d \sin\theta = n\lambda, \quad n \in \mathbb{Z}_+$

Particle in a Box

Standing Wave Condition $\lambda_n = 2L/n, \quad n \in \mathbb{Z}_+$

Energy Level of Particle in a Box

$$E_n = \frac{\pi^2 n^2}{2mL^2}$$

Uncertainty Principle

Uncertainty Principle For non-commutative quantity $[A, B]$, there is

$$\Delta A \Delta B \geqslant \frac{1}{2}$$

Atomic Structure

Nuclear Atom

Rutherford Experiment $\rightarrow$ Atom model

α-particle Scattering Cross Section

$$N(\theta) = \frac{N_\alpha n d Z^2 e^4}{4r^2 K^2 \sin^4(\theta/2)}$$

where N_α is the total number, n is the atom density, d is the foil thickness, Z is the atomic number of foil atom, r is the distance between screen and foil, K is the kinematic energy.

Total Energy

$$K = P = \frac{2Ze^2}{r}$$

Closest Distance

$$r = \frac{2Ze^2}{K}$$

Planetary Models

Energy of Hydrogen Atom

$$E = -\frac{e^2}{2r}$$

Atomic Spectra

Spectra Formulation

$$\frac{1}{\lambda} = R(\frac{1}{m^2} - \frac{1}{n^2}), \qquad m < n$$

with **Lyman**: $m = 1$, **Balmer**: $m = 2$, **Paschen**: $m = 3$, **Brackett**: $m = 4$, **Pfunc**: $m = 5$.

Bohr Atom

Orbital Radius

$$r_n = \frac{n^2}{me^2}$$

with $a_0 = r_1 \sim 5.2 \times 10^{-11}\,\mathrm{m} \sim 2.69 \times 10^{-4}\,\mathrm{eV}^{-1}$ and $r_n = a_0 n^2$

Energy Level of Bohr Atom

Energy Level

$$E = -\frac{e^2}{2r_n} = -\frac{1}{2}me^4 \cdot \frac{1}{n^2}$$

where m is the rest mass of electron. And $E_1 = -13.6\,\mathrm{eV}$.

The lowest energy level E_1 is called the **ground state** of the atom, and the higher levels E_n are called **excited states**.
The work needed to remove an electron from an atom in its ground state is called its **ionization energy**.

Rydberg Constant $R = -E_1/2\pi$

The requirement that quantum physics give the same results as classical physics in the limit of large quantum numbers was called by Bohr the **correspondence principle**.

Nuclear Correction

Reduced Mass $m' = mM/(m+M)$
Energy Level

$$E'_n = \frac{m'}{m}E_n = \frac{M}{M+m}$$

where M is the rest mass of nuclei and m is the rest mass of electron.

Quantum Mechanics

Particle in a Box

Solution:

$$\psi_n = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$$

Expectation value of x: $\langle x \rangle = L/2$

Harmonic Oscillator

Energy level:

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

Hydrogen Atom

Complete Set of Commuting Observables

CSCO of single electron: (n, l, m_l, m_s)
Principal $n = 0, 1, 2, \cdots$ with $E_n = E_1/n^2$
Orbital $l = 0, 1, 2, \cdots . n-1$ with $L = \sqrt{l(l+1)}$
Magnetic $m_l = -l, \cdots, 0, \cdots, l$ with $L_z = m_l$
Spin $m_s = \pm 1/2$ with $S = m_s$

Radiative Transitions

Radiative Transitions: $E_m - E_n = \omega$

Selection Rule

Transitions for which $\langle n|x|m\rangle$ is finite are called **allowed transitions**, while those for which $\langle n|x|m\rangle$ is zero are called **forbidden transitions**.

Selection Rules of Dipole Transition

$$\Delta L = \pm 1, \qquad \Delta m_l = 0, \pm 1$$

Normal Zeeman Effect

Electron Magnetic Moment

$$\mu = -\left(\frac{e}{2m}\right) L$$

where L is the angular momentum.

Spin Magnetic Moment

$$\mu_s = -\left(\frac{e}{m}\right) S$$

The z component is just the Bohr Magneton.

Bohr Magneton

$$\mu_B = \frac{e}{2m}$$

Magnetic Energy

$$U_m = m_l \mu_B B$$

Normal Zeeman Effect

$$\omega \to \omega + m_l \mu_B B$$

Many Electron Atoms

Exclusion Principle

Electron is Fermion → each state can contain no more than one electron

Shell and Subshell

Electrons that share a certain value of n in a shell are said to occupy the same **shell**.
Electrons that share a certain value of l in a shell are said to occupy the same **subshell**.

Hund's Rule

The electrons in a subshell remain unpaired for ground state atom.

Spin-orbit Coupling

Spin-orbit Coupling

$$E_n \to E_n + m_l \mu_B B$$

Total Angular Momentum

> Total Angular Momentum $J = L + S, \quad j = l + s$
> Term Symbol ${}^{2S+1}L_J$

K-series X-ray Spectra

K-series: $E = (10.2\,\text{eV})(Z-1)^2$
Auger Effect: When an electron from an outer shell of an atom with a missing inner electron drops to fill the vacant state, the excitation energy can be carried off by an x-ray photon or by another outer electron. The latter process is called the Auger effect.

Selection Rules

> **Selection Rules of Dipole Transition**
>
> $$\Delta J = 0, \pm 1, \quad J = 0 \not\leftrightarrow 0, \quad \Delta m_J = 0, \pm 1$$

Molecule

> Covalent bound and ionic bound
> Spin of Electron has to be antiparallel in hydrogen atom
> Rotational Energy Levels:
>
> $$E_j = \frac{j(j+1)}{2I}$$
>
> with $I = m'R$ and $m' = m_1 m_2/(m_1 + m_2)$
> Vibrational Energy Levels:
>
> $$E_v = (v + \frac{1}{2})\sqrt{\frac{k}{m'}}$$
>
> where k is a constant.
> Spectra Selection Rules: $\Delta j = \pm 1, \quad \Delta v = \pm 1$

Nuclear Structure

Nuclides $^{A}_{Z}X$ with X chemical symbol of the element, A mass number of the nuclide, Z atomic number of the element

Nuclear Radii $R = R_0 A^{\frac{1}{3}}$ with $R_0 \sim 1.2\,\mathrm{fm}$

Nuclear Magneton

$$\mu_N = \frac{e}{2m_p}$$

with proton $\mu_p z = \pm 2.793\mu_N$ and neutron $\mu_n z = \mp 1.913\mu_N$

Binding Energy The energy equivalent of the missing mass of a nucleus is called the binding energy of the nucleus. The binding energy per nucleon for a given nucleus is an average found by dividing

its total binding energy by the number of nucleons it contains.