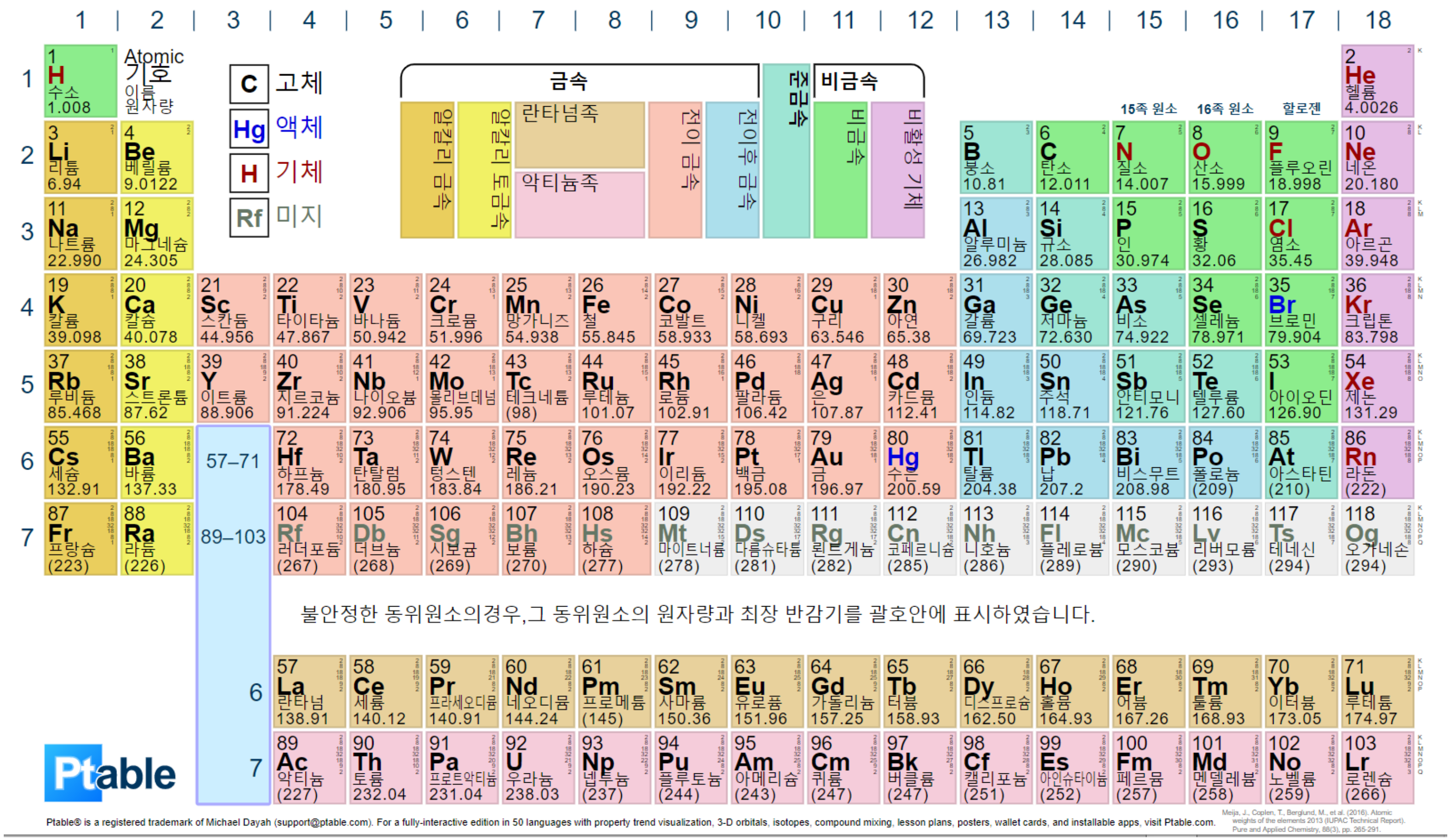
나노소재합성개론

2025-2

Preface to Nanotechnology: Principles and Practices

Atom : 118 elements in periodic table

주기율표



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H 수소 1.008	Atomic 기호 이름 원자량																2 He 헬륨 4.0026
2	3 Li 리튬 6.94	4 Be 베릴륨 9.0122											5 B 붕소 10.81	6 C 탄소 12.011	7 N 질소 14.007	8 O 산소 15.999	9 F 플루오린 18.998	10 Ne 네온 20.180
3	11 Na 나트륨 22.990	12 Mg 마그네슘 24.305											13 Al 알루미늄 26.982	14 Si 규소 28.085	15 P 인 30.974	16 S 황 32.06	17 Cl 염소 35.45	18 Ar 아르곤 39.948
4	19 K 칼륨 39.098	20 Ca 칼슘 40.078	21 Sc 스칸듐 44.956	22 Ti 타이타늄 47.867	23 V 바나듐 50.942	24 Cr 크로뮴 51.996	25 Mn 망가니즈 54.938	26 Fe 철 55.845	27 Co 코발트 58.933	28 Ni 니켈 58.693	29 Cu 구리 63.546	30 Zn 아연 65.38	31 Ga 갈륨 69.723	32 Ge 저마늄 72.630	33 As 비소 74.922	34 Se 셀레늄 78.971	35 Br 브로민 79.904	36 Kr 크립톤 83.798
5	37 Rb 루비듐 85.468	38 Sr 스트론튬 87.62	39 Y 이트륨 88.906	40 Zr 지르코늄 91.224	41 Nb 나이오븀 92.906	42 Mo 몰리브데넘 95.95	43 Tc 테크네튬 (98)	44 Ru 루테늄 101.07	45 Rh 로듐 102.91	46 Pd 팔라듐 106.42	47 Ag 은 107.87	48 Cd 카드뮴 112.41	49 In 인듐 114.82	50 Sn 주석 118.71	51 Sb 안티모니 121.76	52 Te 텔루륨 127.60	53 I 아이오딘 126.90	54 Xe 제논 131.29
6	55 Cs 세슘 132.91	56 Ba 바륨 137.33	57–71	72 Hf 하프늄 178.49	73 Ta 탄탈럼 180.95	74 W 텅스텐 183.84	75 Re 레늄 186.21	76 Os 오스뮴 190.23	77 Ir 이리듐 192.22	78 Pt 백금 195.08	79 Au 금 196.97	80 Hg 수은 200.59	81 Tl 탈륨 204.38	82 Pb 납 207.2	83 Bi 비스무트 208.98	84 Po 폴로늄 (209)	85 At 아스타틴 (210)	86 Rn 라돈 (222)
7	87 Fr 프랑슘 (223)	88 Ra 라듐 (226)	89–103	104 Rf 러더포듐 (267)	105 Db 더브늄 (268)	106 Sg 시보귬 (269)	107 Bh 보륨 (270)	108 Hs 하슘 (277)	109 Mt 마이트너륨 (278)	110 Ds 다름슈타튬 (281)	111 Rg 뢴트게늄 (282)	112 Cn 코페르니슘 (285)	113 Nh 니호늄 (286)	114 Fl 플레로븀 (289)	115 Mc 모스코븀 (290)	116 Lv 리버모륨 (293)	117 Ts 테네신 (294)	118 Og 오가네손 (294)

C 고체

Hg 액체

H 기체

Rf 미지

금속: 알칼리 금속, 알칼리 토금속, 란타넘족, 악티늄족, 전이 금속, 전이후 금속

준금속

비금속: 비금속, 비활성 기체

15족 원소 | 16족 원소 | 할로젠

불안정한 동위원소의경우,그 동위원소의 원자량과 최장 반감기를 괄호안에 표시하였습니다.

6	57 La 란타넘 138.91	58 Ce 세륨 140.12	59 Pr 프라세오디뮴 140.91	60 Nd 네오디뮴 144.24	61 Pm 프로메튬 (145)	62 Sm 사마륨 150.36	63 Eu 유로퓸 151.96	64 Gd 가돌리늄 157.25	65 Tb 터븀 158.93	66 Dy 디스프로슘 162.50	67 Ho 홀뮴 164.93	68 Er 어븀 167.26	69 Tm 툴륨 168.93	70 Yb 이터븀 173.05	71 Lu 루테튬 174.97
7	89 Ac 악티늄 (227)	90 Th 토륨 232.04	91 Pa 프로트악티늄 231.04	92 U 우라늄 238.03	93 Np 넵투늄 (237)	94 Pu 플루토늄 (244)	95 Am 아메리슘 (243)	96 Cm 퀴륨 (247)	97 Bk 버클륨 (247)	98 Cf 캘리포늄 (251)	99 Es 아인슈타이늄 (252)	100 Fm 페르뮴 (257)	101 Md 멘델레븀 (258)	102 No 노벨륨 (259)	103 Lr 로렌슘 (266)

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Meija, J., Coplen, T., Berglund, M., et al. (2016). Atomic weights of the elements 2013 (IUPAC Technical Report). Pure and Applied Chemistry, 88(3), pp. 265-291.

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Preface to Nanotechnology: Principles and Practices

Materials

by combination of different elements in certain proportions, nature has produced a number of gases, liquids, minerals and above all, the living world

Mankind too, ingeniously working, learnt to make a large number of materials and even cast or shape them for desired functions or operations. Starting with stone implements man learnt to separate metals and make alloys. He made wonderful organic and inorganic materials.

use wood, metals, alloys, polymers etc.

directly taken from the nature and some are man-made

Preface to Nanotechnology: Principles and Practices

Materials nowadays

All the materials used today have a variety of functions, which is the fruit of skill and intellect of many generations of mankind.

All this has led to wonderful electronic systems, communication tools, transport vehicles, textile, utensils, architectural materials, medicines etc.

Why mankind has been used materials and tried to develop?

Mankind has been constantly trying to overcome its physical limitations

How? by inventing the appropriate materials and understanding nature's aviation system, man has been able to develop vehicles that run faster than a horse and fly in the sky reaching a height impossible for a bird. He has developed the communication and navigation systems, which take him or his instruments to distant planets. He may not physically go everywhere but he has tried ingeniously to get some knowledge of different planets, stars or even the galaxies.

Preface to Nanotechnology: Principles and Practices

For further development

Man needs more and more materials with controlled properties. He needs materials not known before. He needs materials, which are highly efficient, often small in size and novel.

- In the attempt of making lightweight and smaller and smaller electronic devices, scientists have reduced the size of materials to such an extent that it has reached nanometric dimensions.

At such a scale new phenomena are observed for practically all the materials known so far, leading to novel devices and potential applications in different fields from consumer goods to health related equipment.

Preface to Nanotechnology: Principles and Practices

History of Nanomaterials

Box 1: Milestones in Nanotechnology

- 1857—Michael Faraday synthesized gold colloids of nanosize
- 1915—W. Ostwald, a famous chemist, wrote a book ‘World of Neglected Dimensions’ in German
- 1931—E. Ruska and M. Knoll developed the first electron microscope
- 1951—E. Müller developed the Field Ion Microscope which enabled the imaging of atoms from the tip of metallic samples
- 1959—R. Feynman delivered his now very famous talk ‘There is Plenty of Room at the Bottom’ pointing out to the scientists that reduced dimensionality of materials would create fascinating materials
- 1968—A.Y. Cho and J. Arthur developed Molecular Beam Epitaxy technique for layer by layer growth of materials
- 1970—L. Esaki demonstrated the quantum size effect (QSE) in semiconductors
- 1980—A.I. Akimov showed QSE in CdS and CdSe particles dispersed in glass, triggering the research on nanoparticles
- 1981—G. Binnig and H. Rohrer developed the scanning tunnelling microscope (STM) by which atomic resolution could be obtained. This was also followed by a family of scanning probe microscopes of various types
- 1985—R.F. Curl, H.W. Kroto and R.F. Smalley synthesized sixty atom carbon molecule, later named as ‘Fullerene’
- 1989—D.M. Eigler wrote letters ‘IBM’ using xenon atoms
- 1991—S. Iijima discovered ‘carbon nanotubes’
- 1999—C.A. Mirkin developed the ‘Dip Pen Lithography’
- 2000—D.M. Eigler devised ‘Quantum Mirage’ using Fe atoms on the copper substrate.

Preface to Nanotechnology: Principles and Practices

Beginning of Nanotechnology, Nanoscience

The terms ‘Nanotechnology’ and ‘Nanoscience’ are often used synonymously. The literal meaning of ‘nano’ is ‘dwarf(난쟁이)’ or an abnormally short person. However in scientific language it is a billionth (10^9) part of some unit scale, e.g. nanometre or nanosecond mean 10^9 m or 10^9 s respectively.

Box 2

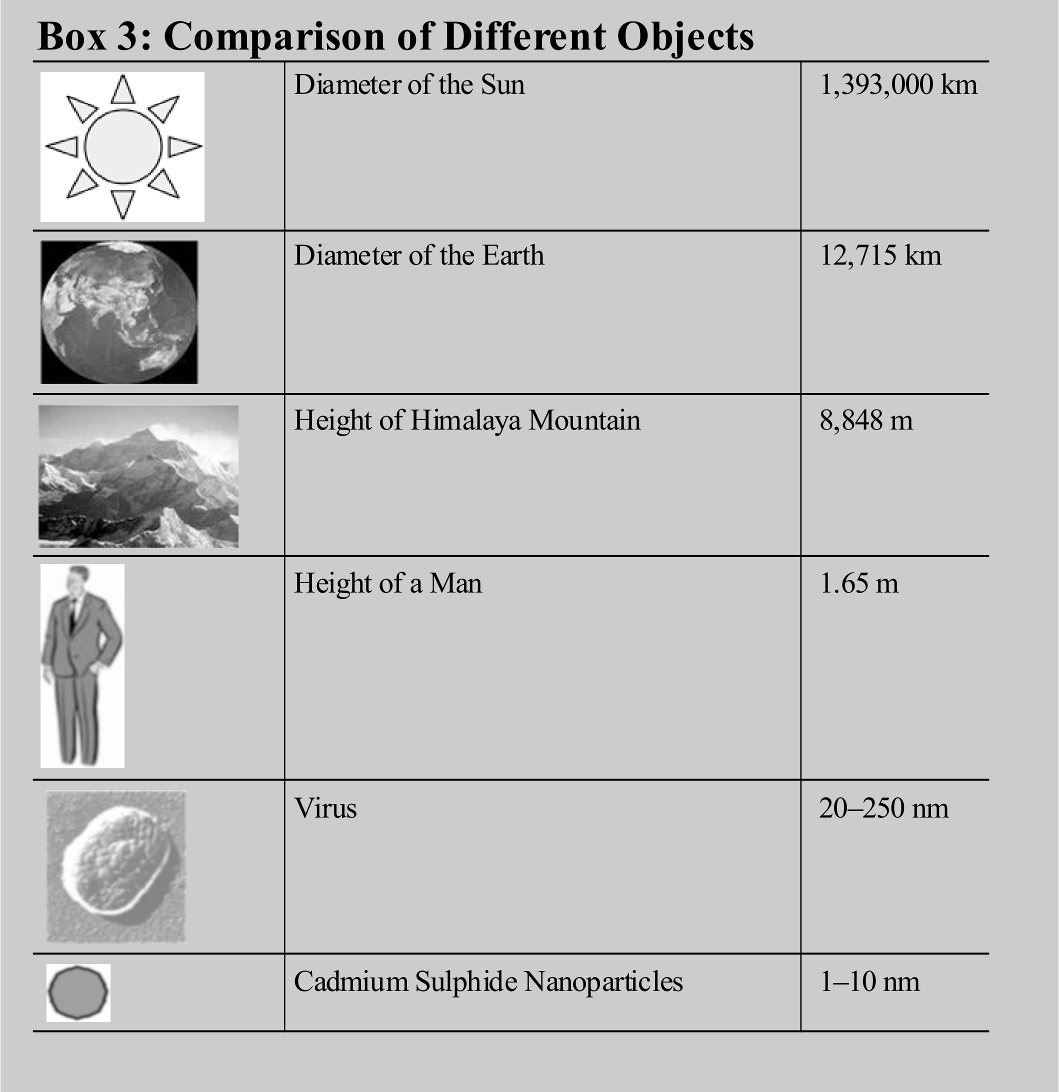
Factor	**Symbol**	**Prefix**	**Factor**	**Symbol**	**Prefix**
10^{18}	a	atto	10^1	da	deka
10^{15}	f	femto	10^2	h	hecto
10^{12}	p	pico	10^3	k	kilo
10^9	n	nano	10^6	M	mega
10^6	μ	micro	10^9	G	giga
10^3	m	milli	10^{12}	T	tera
10^2	c	centi	10^{15}	p	peta
10^1	d	deci	10^{18}	E	exa

Nanometre is so small that if you imagine only ten atoms of hydrogen placed in a line touching each other it will measure one nanometre.

Preface to Nanotechnology: Principles and Practices

Beginning of Nanotechnology, Nanoscience

a qualitative idea on nanometre



Box 3: Comparison of Different Objects

	Diameter of the Sun	1,393,000 km
	Diameter of the Earth	12,715 km
	Height of Himalaya Mountain	8,848 m
	Height of a Man	1.65 m
	Virus	20–250 nm
	Cadmium Sulphide Nanoparticles	1–10 nm

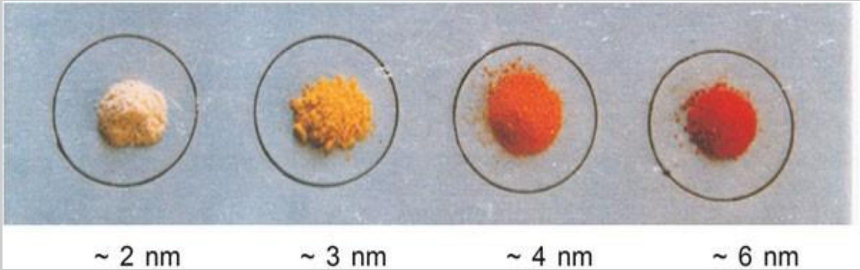
Preface to Nanotechnology: Principles and Practices

Nanotechnology

Nanotechnology is thus the technology of materials dealing with very small dimension materials usually in the range of 1–100 nm.

- When at least one of the dimensions of any type of material is reduced below 100 nm, its mechanical, thermal, optical, magnetic and other properties change at some size characteristic of that material. Thus within the same material one can get a range of properties.

Box 4: CdS Nanoparticles (Colour Change with Particle Size)



Not only the visual appearance but other properties also change dramatically.
Melting point for pure bulk solids is very sharply defined.
the melting point reduces with the particle size.
Therefore by changing the particle size of a material one can achieve a range of properties

Preface to Nanotechnology: Principles and Practices

Nanotechnology

Nanotechnology is an interdisciplinary science. It needs Physics, Chemistry, Engineering, Biology etc. so that its full potential can be exploited for the advantage of mankind.

What has been achieved in nanotechnology so far is only the tip of the iceberg.

To fully explore the potential of nanotechnology it is essential to know what are nanomaterials, how and why do they differ from other materials, how to synthesize/analyze the nanomaterials organize them and understand some already proven application areas.

What we are going to learn!

1. Introduction to Quantum Mechanics

1. Introduction to Quantum Mechanics

1.1 Why quantum mechanics?

Nanotechnology we are concerned with natural and synthetic materials in the size range of 1–100 nm.

➡ Classical, Newtonian mechanics or thermodynamics are not able to explain the observed properties of materials.

[Box 1.1] some historical milestones, which have led to quantum mechanics

Box 1.1: Historical Milestones in the Development of Quantum Mechanics Pre-quantum Era

- In 1669, Newton proposed that light had corpuscular or particle nature.
- Huygen claimed in 1690 that light had a wave nature.
- Kirchoff and others studied black body radiation around 1860.
- Maxwell proposed (1873) theory of electromagnetic waves.
- In 1803–04 Young performed double slit experiment, which showed that light had a wave nature.
- In 1887, Heinrich Hertz produced and detected electromagnetic radiation.

(continued)

1. Introduction to Quantum Mechanics

Box 1.1 (continued)

Old Quantum Theory Period

- In 1901, Max Planck showed that energy distribution in black body radiation could be explained properly only if one considered that the radiation was quantized or had a particle nature.
- In 1905, Einstein proposed a theory of photoelectric effect which decisively proved that quantum or particle nature was associated with electromagnetic waves.
- Compton effect (1920) could be explained only when particle nature of electromagnetic radiation was considered, supporting Max Planck’s and Einstein’s theories. Particles of electromagnetic waves were identified as ‘photons’.
- De Broglie (1923) argued that if electromagnetic waves were particles (photons) then why not particles have waves associated with them?
- Bohr’s atom model (1913) with stationary states (why electrons should have some fixed energies) could be explained with de Broglie hypothesis.

Modern Quantum Theory Begins

- Heisenberg introduced (1925) Matrix Mechanics.
- Schrödinger equation (1926) gave the firm foundation for de Broglie hypothesis and later explained the electronic structure of atoms, molecules and solids.
- Davisson and Germer showed in 1927 that electrons can be diffracted. Regularly spaced atoms constitute multi-slit analogue of Young’s double slit experiment.
- Heisenberg proposed uncertainty principle in 1928.

This marks the beginning of Quantum Mechanics as it is practiced now!

1. Introduction to Quantum Mechanics

- Black body radiation

When any radiation is incident on a body, what will it do? It will either reflect (r), absorb (a) or transmit (t), though partially, so that r + a + t = 1. A material is called a 'black body'

Box 1.3: Black Body Radiation
All materials absorb and emit energy. The intensity of energy radiated and absorbed by a body are equal if the object is in thermal equilibrium with its surrounding. However if the body is above the temperature of its surrounding then it emits radiation, which is known as black body radiation. Black body is thus an object that can absorb all radiation incident on it (no reflection or transmission!) or emits all radiation when above the temperature of the surrounding. Typical black body spectra are illustrated in Fig. 1.1.

Total intensity of radiation (area under the curve) and intensities at different emission wavelengths of a perfect black body irrespective of its material depend on the temperature. In practice a cavity with a small hole can act like a black body.

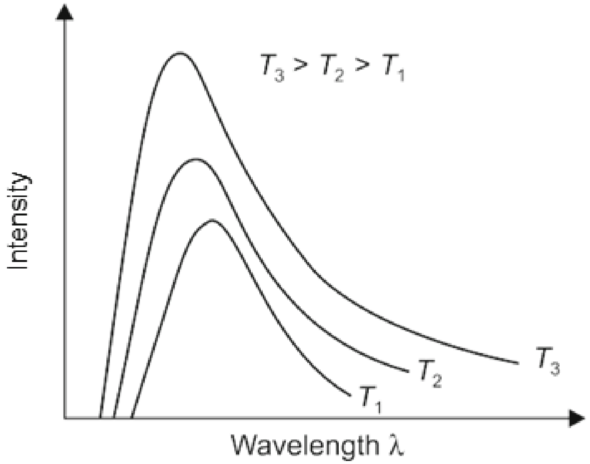


Fig. 1.1 Spectra of Black body radiation. Note that as the temperature increases, the spectral intensity increases and maximum intensity shifts to shorter wavelength. T_1, T_2 and T_3 are different temperatures in the increasing order

1. Introduction to Quantum Mechanics

- Black body radiation

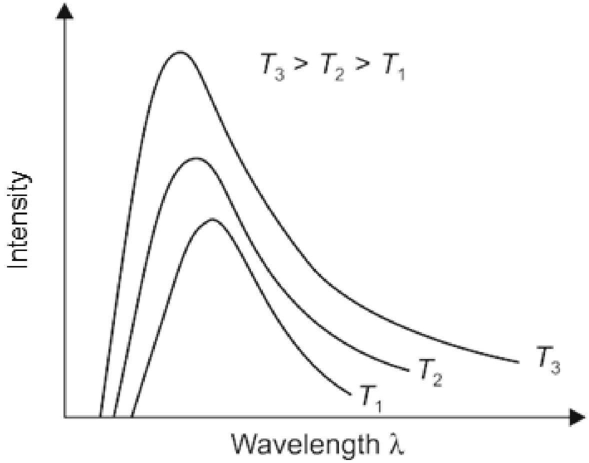
If it absorbs all radiation incident on it without reflecting or transmitting it. When a black body is heated, it gives out a spectrum as shown in Fig. 1.1. The black body spectrum spreads over a large range of wavelengths and has a maximum in the intensity.

Experiments on black body radiation led Stefan (1879) and Boltzman (1884) to establish Stefan-Boltzman law.

*According to this law, the total radiation from a black body is proportional to the fourth power of absolute temperature

$$E = \sigma T^4$$

E: the intensity of total radiation,
T: the absolute temperature
σ: Stefan's constant ($\sigma = 5.669 \times 10^8$ W/m^2)



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1. Introduction to Quantum Mechanics

- Black body radiation (by Wien)

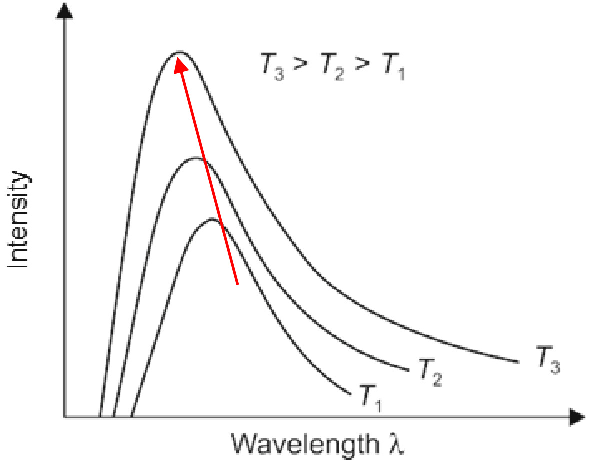
As the temperature of the black body increased, the maximum in the black body spectrum shifted to shorter wavelength or higher energy

! Compare charcoal or iron.

- At room temperature, they look black.

- If we heat these materials then what happens? First they look faint red, then they change to bright red and then become bright yellow or white.

“Wavelength is getting shorter”



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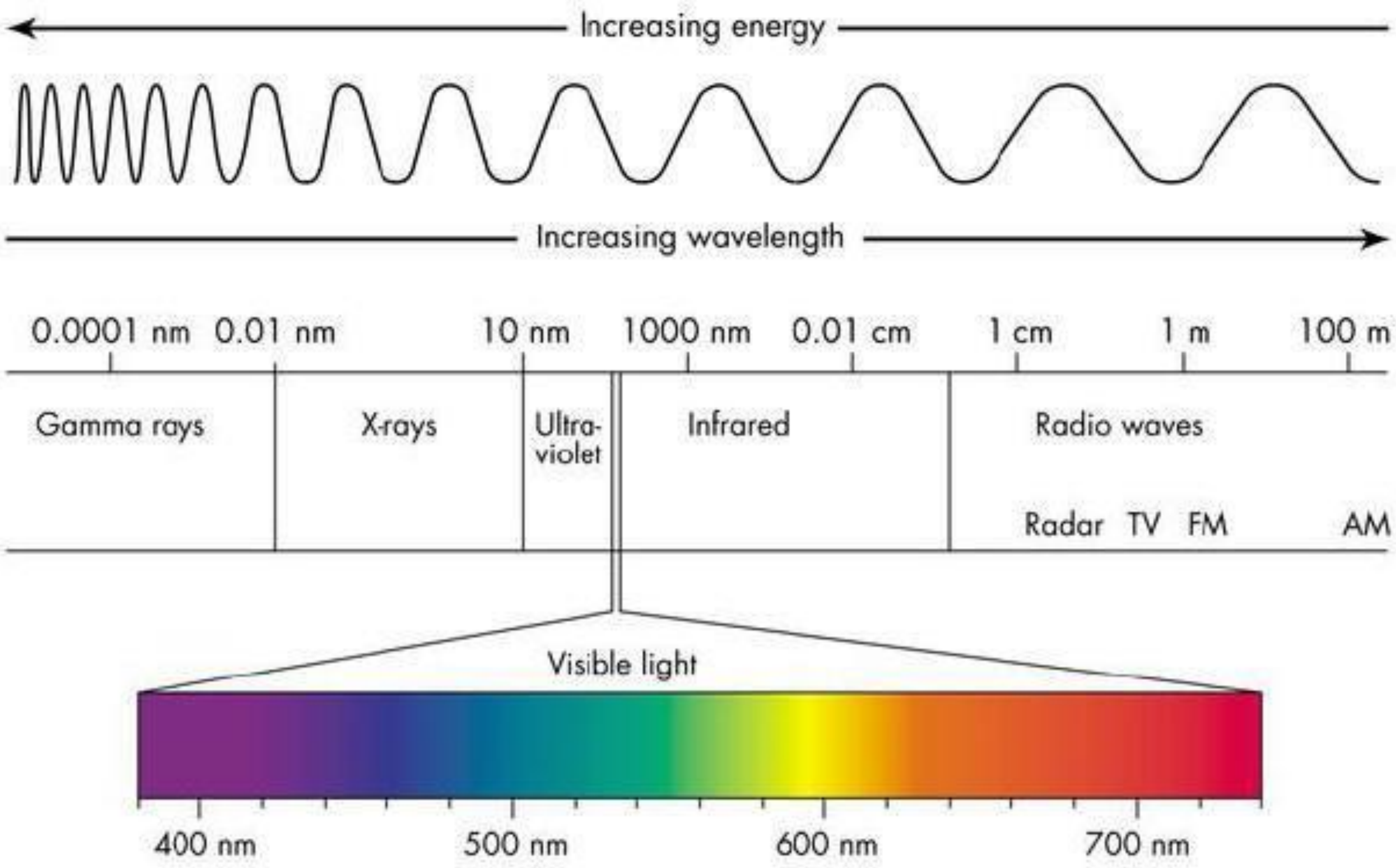
1. Introduction to Quantum Mechanics

- Wavelength vs Color



1. Introduction to Quantum Mechanics

- Black body radiation (by Wien)

Wien’s precise experiments on black body radiation resulted into a law

$$\lambda_{\max} \times T = \text{Wien displacement constant} \cong 2.898 \times 10^{-3} \ \text{mK}$$

$\lambda_{\max}$ is the wavelength at which maximum intensity occurs for a black body held at temperature T

The intensity varied with wavelength as

$$E_\lambda = \frac{a}{\lambda^5} \exp\left(\frac{-b}{\lambda T}\right)$$

Total energy radiated per unit time, per unit surface area is given by

$$E = \int_0^\infty E_\lambda d\lambda$$

$E_\lambda d\lambda$ is the rate of energy emission per unit area in the wavelength range λ to $\lambda + d\lambda$

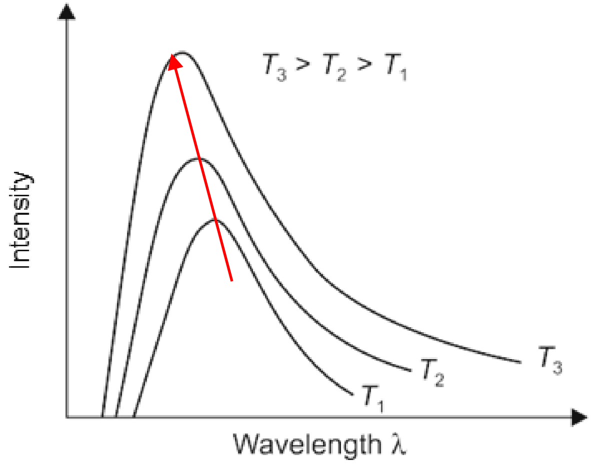


Fig. 1.1 Spectra of Black body radiation. Note that as the temperature increases, the spectral intensity increases and maximum intensity shifts to shorter wavelength. T_1, T_2 and T_3 are different temperatures in the increasing order

➡ This formula holds good only for short wavelength side of the spectrum

1. Introduction to Quantum Mechanics

- Black body radiation (by Rayleigh and Jean)

$$E_\lambda = \frac{2c}{\lambda^4} kT$$

'*c*' is velocity of light
'*k*' is Boltzman constant

*This equation could explain the <u>long wavelength side</u> of the black body spectrum <u>not for short wavelength</u>

- Black body radiation (by Planck, 1901)

$$E_\lambda = \frac{2\pi hc^2}{\lambda^5} \frac{1}{\left(e^{hc/\lambda KT} - 1\right)}$$

'*h*' is Planck's constant

Planck proposed that radiation cannot be absorbed or emitted continuously.

<u>The absorption or emission of radiation through some quantum of energy or 'quanta' like particles, later termed as **photons**.</u>

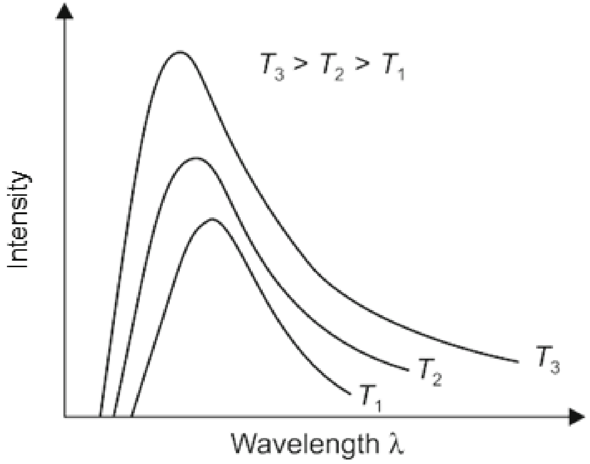


Fig. 1.1 Spectra of Black body radiation. Note that as the temperature increases, the spectral intensity increases and maximum intensity shifts to shorter wavelength. T_1, T_2 and T_3 are different temperatures in the increasing order

1. Introduction to Quantum Mechanics

- Black body radiation (by Planck, 1901)

$$E_\lambda = \frac{2\pi hc^2}{\lambda^5}\frac{1}{(e^{hc/\lambda KT}-1)}$$

'*h*' is Planck's constant

Energy of each quantum of radiation (absorbed or emitted) was assumed to be hυ, where υ is the frequency of absorbed or emitted radiation.

The total radiated energy

$$E = \frac{2\pi^5 k^4}{15c^2h^3}T^4$$

- This equation is valid at short and long wavelengths equally.

Planck's equation successfully explained all the regions of Black Body spectrum as well as previous findings and laws

Planck's idea that electromagnetic radiation should be considered as quantum of radiation turned out to be a milestone in the development of modern science

1. Introduction to Quantum Mechanics

Box 1.4: Max Planck (1858–1947)

Max Planck was born in Kiel, Germany, in the year 1858. He studied physics in Munich as well as Berlin, Germany. He became a Professor of Theoretical Physics in 1892 in Berlin University. There he discovered in 1899 the fundamental constant '*h*' or Planck's constant named after him. Immediately in 1900 he discovered what is known now as 'Planck's law of black body radiation'.

This law became the foundation of quantum theory. Max Planck was awarded the Nobel Prize for Physics in 1918. From 1930 to 1937, Planck was head of the Kaiser Wilhelm Gesellschaft zur Fördernen der Wissenschaften (KWG, Emperor Wilhelm Society for the Advancement of Science) which was renamed after his death on 4th October 1947 in Götingen, Germany as Max Planck Gesellschaft zur Förderung der Wissenschaften (MPG, Max Planck Society for the Advancement of Science). This institute continues to be one of the most important institutes for science in Germany.

1. Introduction to Quantum Mechanics

- Assumption on the existence of photons or quanta of electromagnetic radiation

➡ 1. Photoelectric effect
2. Compton effect

1. Photoelectric effect

Box 1.5: Photoelectric Effect
If two metal electrodes are placed in an evacuated tube, separated by a short distance, as illustrated in Fig. 1.2a then current flows in the circuit if cathode is irradiated with UV to visible light. This is known as photoelectric effect. It is easy to understand that the circuit is completed if electrons are emitted from cathode reaching the anode on illumination of the cathode. Einstein successfully explained in 1905 the observations by assuming that the incident beam of light behaved like photons or quanta of radiation proposed by Max Planck.

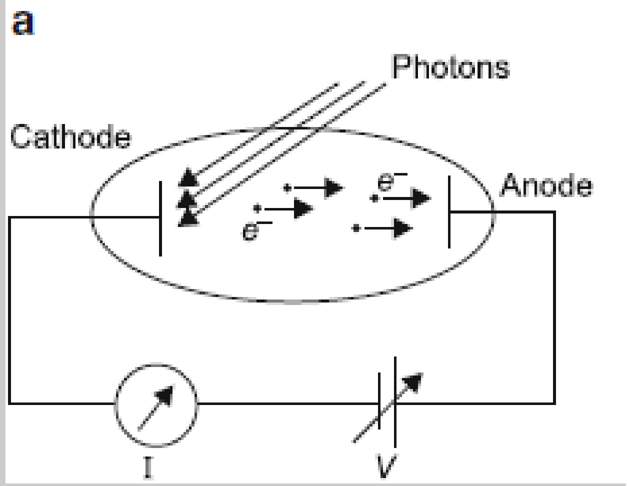


Fig. 1.2 (**a**) Circuit diagram to observe photoelectric effect

1. Introduction to Quantum Mechanics

1. Photoelectric effect

1. Photoelectric current (I) is proportional to the intensity of light (Int) falling on the cathode (see Fig. 1.2b).
2. There exists a threshold frequency dependent on the cathode material, which is necessary to emit photoelectrons. If light of lesser frequency is used then, even for any high intensity, no photoelectrons can be emitted.
3. This implies that there is a maximum kinetic energy which is necessary to produce photoelectric current.

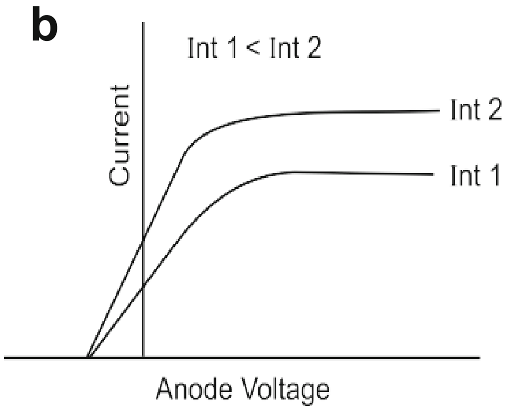


Fig. 1.2 (**b**) Variation of current due to photoelectrons. Here 'Int' is the intensity of light

$$k_{\max} = eV_0 = \frac{1}{2}mv^2$$

where V_0 is the stopping potential, *e* and *m* are electron charge and mass respectively. The velocity is *v*.

Even if anode is negative (V_0), electrons with maximum kinetic energy eV_0 can reach the anode.

Maximum energy of emitted photoelectrons does not depend upon the intensity of incident light but the frequency used as illustrated in Fig. 1.3.

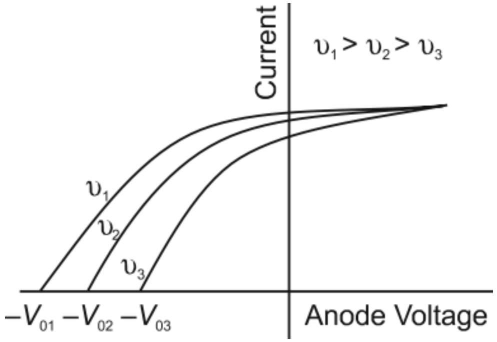


Fig. 1.3 Negative anode voltage V_0 denotes the maximum kinetic energy the electrons can have in a photoemission process. It depends on the frequency υ of the incident light

4. Emitted photoelectrons have maximum energy (corresponding to $-V_0$) which depends upon the **frequency** of incident light.

1. Introduction to Quantum Mechanics

1. Photoelectric effect

Number of ejected photoelectrons depends upon the intensity of light but the maximum kinetic energy of ejected photoelectrons depends upon the frequency of light. There is a minimum frequency ‘υ_0’ necessary to eject the photoelectrons which depends upon the material. This can be stated as

$$\text{Maximum kinetic energy} = h\upsilon - h\upsilon_0$$

where $h\upsilon$ is the energy larger than minimum energy $h\upsilon_0$ required to eject the photoelectron (Fig. 1.4).

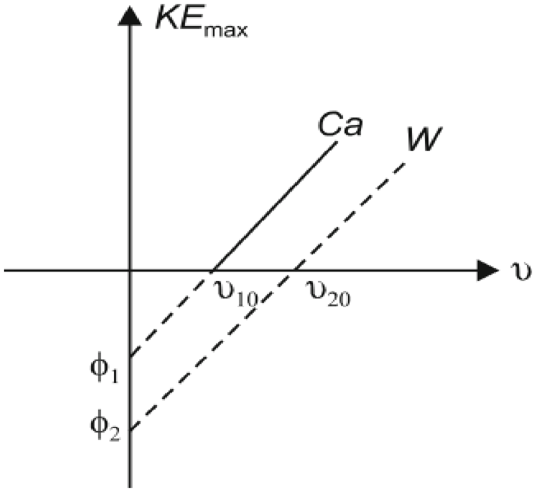


Fig. 1.4 Maximum kinetic energy depends upon the frequency of incident light and the material of cathode. Note that the lines have same slope (see Eq. 1.9). Here Ca and W are calcium and tungsten cathodes respectively. Φ_1 and Φ_2 are work functions of Ca and W respectively. **Work function is a property of the material and denotes the amount of energy required to remove the electron from that material**

1. Introduction to Quantum Mechanics

- Assumption on the existence of photons or quanta of electromagnetic radiation

1. Photoelectric effect
2. Compton effect

2. Compton effect

Box 1.6: Compton Scattering
X-rays with sufficiently high energy, when incident on a stationary electron as Compton imagined in 1920, can change their own direction as well as wavelength to longer side, reducing their energy. Reduced energy is imparted to the electron which gains a momentum *p*=*mv* where *m* is the mass of the electron and *v* is the velocity gained by the electron.

$$\text{K.E of electron} = h\upsilon - h\upsilon'$$

where υ and υ' are the frequencies of incident X-rays before and after scattering

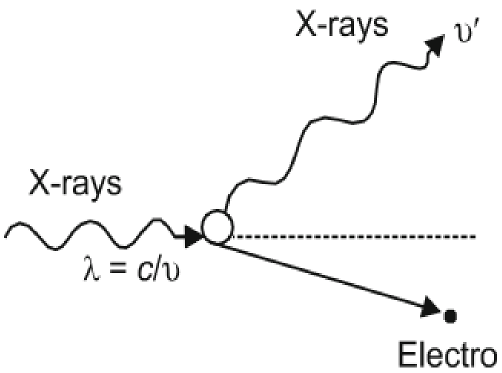


Fig. 1.5 Schematic of Compton effect $\upsilon < \upsilon'$

From conservation of momentum, <u>momentum gained by the electron must be same as that lost by X-rays</u> or we need to assume that X-rays which are electromagnetic waves have momentum $p = h/\lambda$ and <u>X-rays behave as particles or photons</u>.

1. Introduction to Quantum Mechanics

- Wave-particle duality

<Particle>

Einstein's theory of photoelectric effect and Compton effect could be explained only if one assumed the existence of photons or quanta of electromagnetic radiation.

<Wave>

Electromagnetic radiation also exhibits interference of light. This is quite evident from Young's diffraction experiments with single and double slits.

➡ Depends upon the type of experiment that electromagnetic radiation shows itself as waves or particles. **Waves are continuous and particles are discrete** in nature.

The behaviour of electromagnetic waves sometimes as waves and sometimes as particles is termed as 'wave-particle duality'

1. Introduction to Quantum Mechanics

1.2 Matter Waves（물질파）

- From wave-particle duality of electromagnetic wave….

if electromagnetic waves sometimes behave like particles (photons) then why not particles behave like waves?

- de Broglie in 1923

postulated that all the matter must have associated waves with wavelength given by

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

where h = Planck's constant, p = magnitude of the momentum, m = mass of the particle and v = velocity of the particle.

de Broglie relation and wavelength (λ) is known as de Broglie wavelength of the particle

➡ a very effective way of explaining various properties of atoms and subatomic particles like electrons, protons and neutrons.

"Not go deep inside this lecture"

1. Introduction to Quantum Mechanics

1.3 Heisenberg’s Uncertainty Principle (불확정성의 원리)

- No classical analogue but is one of the basic concepts in quantum mechanics.

If we have a source of monochromatic light (**single wavelength**) at the back of two slits as shown in Fig. 1.6, we would obtain a diffraction pattern i.e. bands of dark and light areas.

Dark bands correspond to the regions where light does not strike and light areas correspond to areas where light is able to reach.

Replace now the source of light with source of mono energetic electrons from an electron gun.

We would get the diffraction pattern of light and dark regions by exposure of photographic plate to electrons.

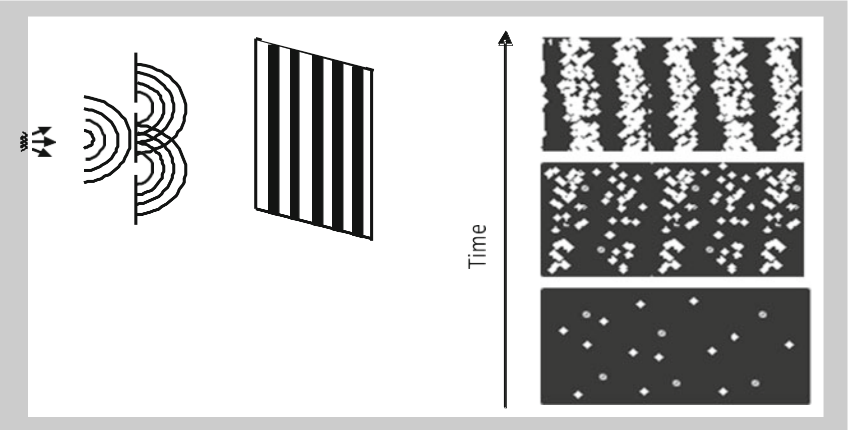


Fig. 1.6 (**a**) Schematic diagram to obtain diffraction pattern (slits S1 and S2) on the photographic plate P (one may use some counter also to detect the intensity). One can use photons or electrons as the source. (**b**) Electron diffraction pattern for change in exposure (counting) time

1. Introduction to Quantum Mechanics

- If we make few more experiments by reducing the electron beam intensity, we can see some interesting effect. What happen?

we would see blurred interference pattern and with further reduction of electron beam intensity we may get only a couple of spots and no bands of light and dark areas.

Electrons appear to have gone to places where intensity maxima appear in diffraction pattern

Very large, precision would be lost and we would not know through which slit the electron came out.

In other words we cannot precisely know position and momentum of the electron simultaneously with arbitrary accuracy.

If we reduce the momentum uncertainty (using long wavelength), position becomes uncertain and if we measure the position with certainty using short wavelength then momentum becomes uncertain destroying the diffraction pattern.

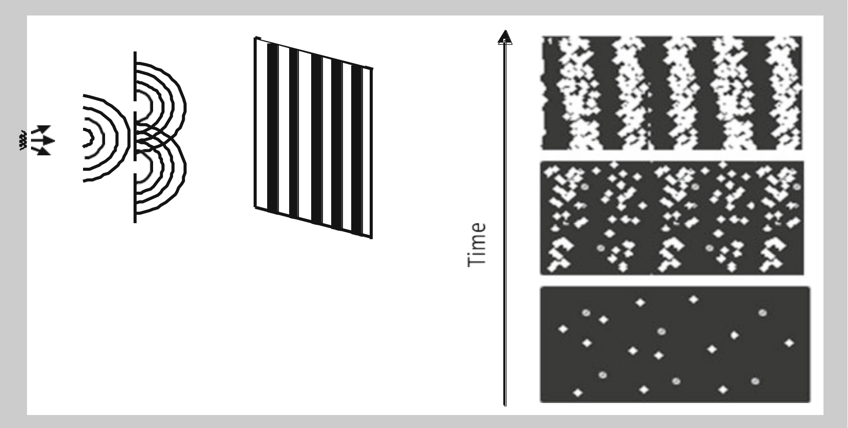


Fig. 1.6 (**a**) Schematic diagram to obtain diffraction pattern (slits S1 and S2) on the photographic plate P (one may use some counter also to detect the intensity). One can use photons or electrons as the source. (**b**) Electron diffraction pattern for change in exposure (counting) time

1. Introduction to Quantum Mechanics

- It is <u>not possible to keep both ***position*** and ***momentum*** measurement precise, simultaneously</u>

Precise measurement of one disturbs the other measurement.

$$\Delta x . \Delta p \geq \frac{h}{2\pi}$$

Δx is the dispersion $\left(= \sqrt{< (x - < x >)^2 >}\right)$ in the measurement of position in x direction and p is the dispersion in the simultaneous measurement of x component of momentum of a particle

In general, Heisenberg's uncertainty principle states that "<u>it is impossible to determine precisely and simultaneously the values of both the members of a particular pair of physical variables such as position components in a particular direction and momentum in that direction</u>, energy of a bound state and its decay time etc."

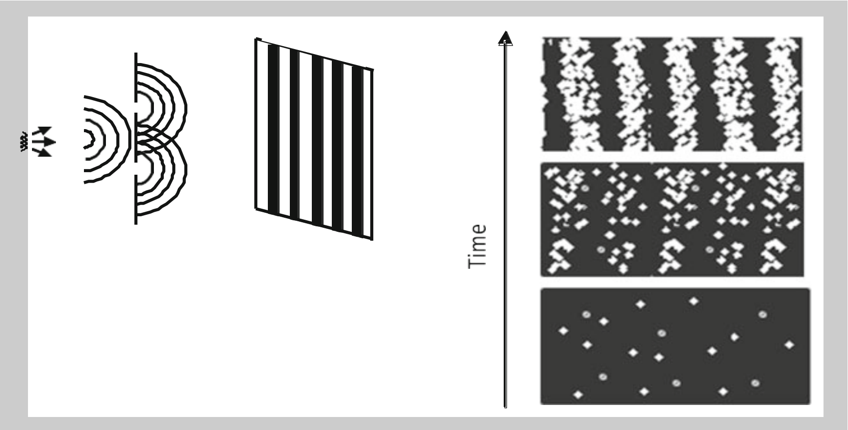


Fig. 1.6 (**a**) Schematic diagram to obtain diffraction pattern (slits S1 and S2) on the photographic plate P (one may use some counter also to detect the intensity). One can use photons or electrons as the source. (**b**) Electron diffraction pattern for change in exposure (counting) time

1. Introduction to Quantum Mechanics

1.4 Schrödinger Equation

- Comparison between classical and quantum mechanics

Classical Mechanics	Quantum Mechanics
1) It deals with macroscopic particles	1) It deals with microscopic or nanoscopic particles
2) It is based upon Newton's laws of motion	2) It takes into account Heisenberg's uncertainty principle and de Broglie concept of dual nature of matter (particle nature and wave nature)
3) It is based on Maxwell's electromagnetic wave theory according to which any amount of energy may be emitted or absorbed continuously	3) It is based on Planck's quantum theory according to which only discrete values of energy are emitted or absorbed
4) The state of a system is defined by specifying all the forces acting on the particles as well as their positions and velocities(moment). The future state then can be predicted with certainty	4) It gives probabilities of finding the particles at various locations in space
The study of forces acting on bodies whether at rest or in motion	The study of the discrete nature of phenomena at the atomic and subatomic level

In classical mechanics, use Newton's equations to determine the position of a given particle under some conditions like its speed, initial velocity etc.

In quantum mechanics, use Schrödinger equation to understand the behaviour of subatomic particles

1. Introduction to Quantum Mechanics

1.4 Schrödinger Equation

For a free particle, in one dimension, time dependent Schrödinger equation is as follows:

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

$\psi(x, t)$ is the wave function of particle of mass m

neglect the potential energy V and assume that

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

the kinetic energy of the particle.

E = kinetic energy + potential energy

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

- One dimensional form of Schrödinger equation

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

1. Introduction to Quantum Mechanics

- Three dimensional form of Schrödinger equation

(put x, y, z axis)

$$\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z,t)+V(x,y,z,t)\,\psi(x,y,z,t)$$

$$=i\hbar\frac{\partial\psi(x,y,z,t)}{\partial t}$$

- We can use Laplacian notation

and **r** for (*x*, *y*, *z*)

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

- <u>Time-dependent</u> Schrödinger equation in <u>three dimensions</u>

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

1. Introduction to Quantum Mechanics

- Time independent Schrödinger equation in one dimension

$$V(x,t) = V(x)$$

*In case the potential energy of a particle does not change with time (as in case of energy states of electrons in an atom)

$$\Rightarrow \quad \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x2} + \boxed{V(x)}\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

Assuming that wave function ψ(*x*, *t*) can be separated into two parts viz. one varying with position and the other with time

$$\psi(x,t) = \Phi(x)\theta(t)$$

$$\frac{-\hbar^2}{2m}\theta(t)\frac{d^2\Phi(x)}{dx^2} + V(x)\Phi(x)\theta(t) = i\hbar\Phi(x)\frac{d\theta(t)}{dt}$$

or

$$\frac{-\hbar^2}{2m\Phi(x)}\frac{d^2\Phi(x)}{dx^2} + V(x) = \frac{i\hbar}{\theta(t)}\frac{d\theta(t)}{dt}$$

only position dependent

only time dependent

1. Introduction to Quantum Mechanics

each side of the equation must be a constant, say A

$$\boxed{\frac{-\hbar^2}{2m\Phi(x)}\frac{d^2\Phi(x)}{dx^2}+V(x)}=\boxed{\frac{i\hbar}{\theta(t)}\frac{d\theta(t)}{dt}}$$

$$\boxed{\begin{aligned}&\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}=i\hbar\frac{\partial\psi(x,t)}{\partial t}\\&E=\frac{\hbar^2k^2}{2m}\end{aligned}}$$

➡ $\frac{-\hbar^2}{2m\Phi(x)}\frac{d^2\Phi(x)}{dx^2}+V(x)=A$ $\quad\frac{i\hbar}{\theta(t)}\frac{d\theta(t)}{dt}=A$

Solve, $\theta(t)=\theta(0)e^{\frac{-iAt}{\hbar}}$ where $\theta(0)$ is $\theta(t)$ at time $t=0$.

From $i\hbar\frac{\partial\psi(x,t)}{\partial t}=E\psi(x,t)$ and $\frac{i\hbar}{\theta(t)}\frac{d\theta(t)}{dt}=A$

at $x=0$. This implies that $A=E$ $\quad\frac{d\theta(t)}{\theta(t)}=-iE\frac{dt}{\hbar}$ Integrating it, $\theta(t)=\exp\left(\frac{-iEt}{\hbar}\right)$

Substituting A with E of $\frac{-\hbar^2}{2m\Phi(x)}\frac{d^2\Phi(x)}{dx^2}+V(x)=A$

➡ One dimensional, time independent Schrödinger equation

$$\boxed{\begin{aligned}&\frac{-\hbar^2}{2m\Phi(x)}\frac{d^2\Phi(x)}{dx^2}+V(x)=E\\\text{or}\quad&\frac{-\hbar^2}{2m}\frac{d^2\Phi(x)}{dx^2}+V(x)\Phi(x)=E\Phi(x)\end{aligned}}$$

1. Introduction to Quantum Mechanics

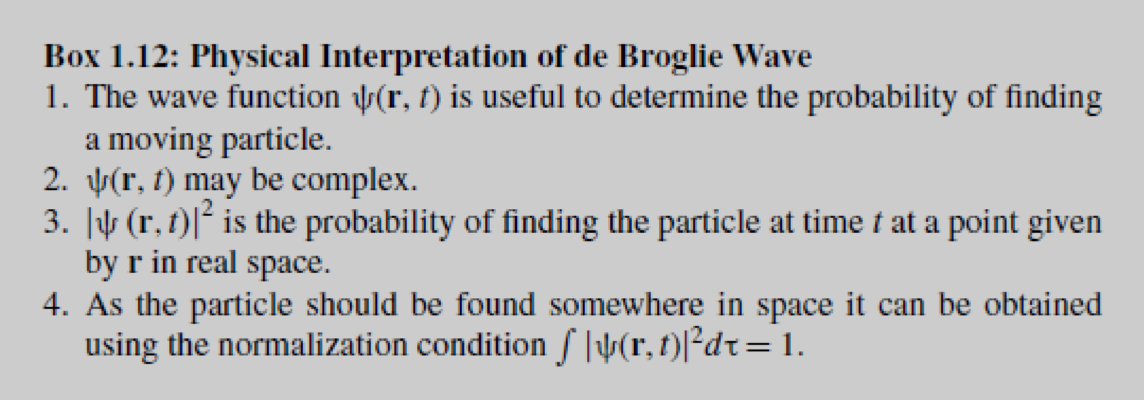
- Three dimensional, time independent Schrödinger equation

$$\psi(\mathbf{r},t) = \psi(\mathbf{r})\,\Phi(t)$$

$$\frac{-\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\,\psi(\mathbf{r}) = E\,\psi(\mathbf{r})$$

In order to determine the energy states of a particle it is necessary to know the form of potential V and how particle amplitude varies in space or $\psi(\mathbf{r})$

There may be a number of wave functions satisfying Schrödinger equation, but all may not be able to describe a given situation.
The acceptable wave function should **satisfy physical boundary conditions**.
It is necessary that ψ should satisfy following conditions so that using Schrödinger equation one can obtain the realistic values of energy



Box 1.12: Physical Interpretation of de Broglie Wave

1. The wave function $\psi(\mathbf{r}, t)$ is useful to determine the probability of finding a moving particle.
2. $\psi(\mathbf{r}, t)$ may be complex.
3. $|\psi(\mathbf{r}, t)|^2$ is the probability of finding the particle at time t at a point given by $\mathbf{r}$ in real space.
4. As the particle should be found somewhere in space it can be obtained using the normalization condition $\int |\psi(\mathbf{r}, t)|^2 d\tau = 1$.

1. Introduction to Quantum Mechanics

1.5 Electron Confinement

Nano structured materials have at least one of the dimensions in the range of 1–100 nm

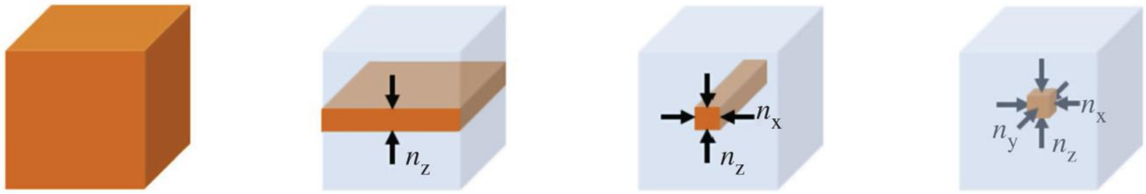
➡ properties of materials can be understood using quantum mechanics

To understand various properties even in case of bulk solids we need to understand the electron properties which are subatomic particles

<Confinement of a particle>

in one (1D) dimension (freedom in 2D),
in two(2D) dimensions (freedom in 1D)
in all three(3D) dimensions (no freedom in any direction or 0D material).

no confinement	1D confinement	2D confinement	3D confinement
bulk	Q-well/ultrathin film	Q-wire	Q-dot
(3D materials)	(2D materials)	(1D materials)	(0D material)



2D quantum wells (thin film)	1D wire (wire)	0D quantum dot (nanoparticles)

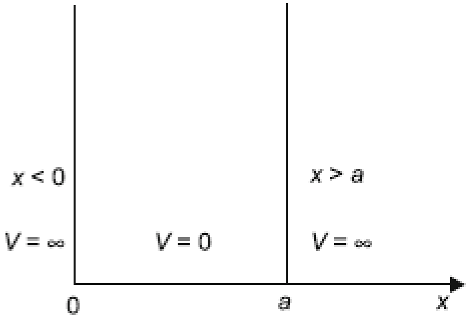
1. Introduction to Quantum Mechanics

1.5.1 Particle in a Box

Consider a box of length '*a*' such that

Potential $V = 0 \quad \text{if } 0 < x < a$

and $V = \infty \quad \text{if } x < 0 \text{ or } x > a$



Energy states of the particle of mass *m* can be obtained using time independent Schrödinger equation for one dimension

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

Let $\psi(x)$ have a general form as

$$\psi(x) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}}x + B\cos\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}}x$$

1. Introduction to Quantum Mechanics

1.5.1 Particle in a Box

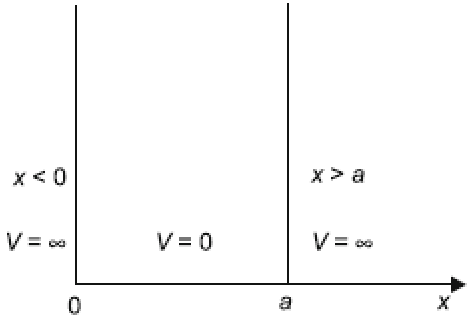


Fig. 1.7 One dimensional potential box

As the particle exists only inside the box, wavefunction should not exist outside the box and should be zero at the boundaries

<Boundary condition>

At $x = 0$, boundary condition $\psi(x) = 0$ leads to $B = 0$.

$$\psi(x) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} x + B\cos\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} x \quad \Rightarrow \quad \psi(x) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} x$$

At $x = a$, boundary condition $\psi(a) = 0$ leads to

$$\psi(x) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} x + B\cos\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} x \quad \Rightarrow \quad \boxed{\psi(a) = 0 = A\sin\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} a}$$

1. Introduction to Quantum Mechanics

1.5.1 Particle in a Box

But 'a' is not zero, $\psi(a) = 0 = A\sin\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} a$

$$\sin\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} a = 0 \quad \text{or,} \quad \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} a = \boxed{n\pi}$$

where $n = 0, 1, 2, 3, \ldots$

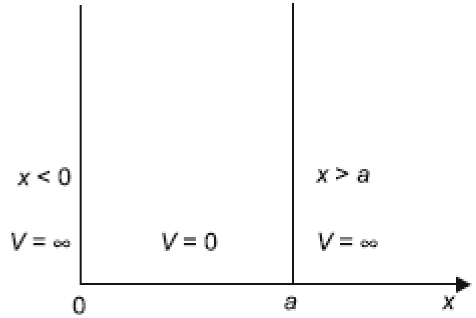
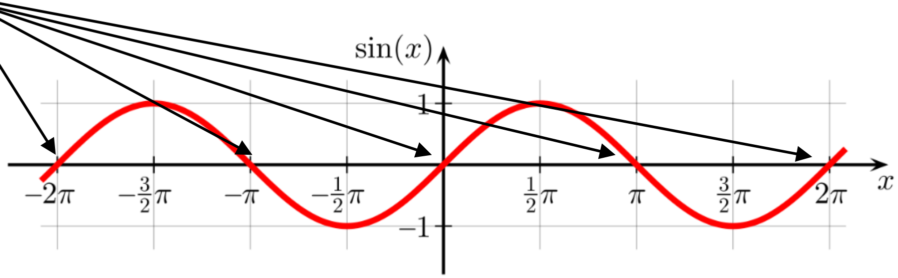


Fig. 1.7 One dimensional potential box



$$\Rightarrow \quad E_n = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2h^2}{8ma^2}$$

$$\psi(x) = A\sin\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} x \quad \Rightarrow \quad \boxed{\psi_n = A\sin\left(\frac{n\pi}{a}\right)x}$$

*입자가 가질 수 있는 허용된 파장이 n 에따라 특정 값으로 결정됨

'n' is quantum number (양자수)

1. Introduction to Quantum Mechanics

1.5.1 Particle in a Box

$$\psi_n = A \sin\left(\frac{n\pi}{a}\right) x$$

*입자가 가질 수 있는 허용된 파장이 n 에따라 특정 값으로 결정됨

'n' is quantum number (양자수)

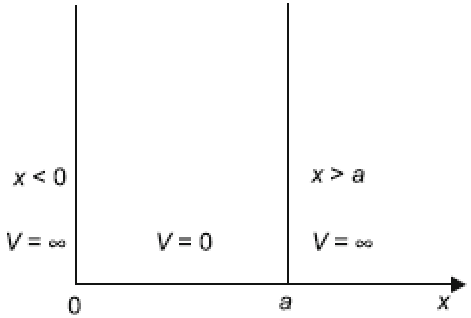


Fig. 1.7 One dimensional potential box

Although n can take any integer value according to $E_n = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2h^2}{8ma^2}$

in practice $n = 0$ and ψ_n=0 are not allowed inside the box.
because, if allowed, $|\Psi|^2$ would be 0 and probability of finding the particle inside the box would be zero.

ψ cannot be zero inside the box. Therefore n takes the values $n = 1, 2, 3, \ldots\ldots$

1. Introduction to Quantum Mechanics

1.5.1 Particle in a Box

$$E_n = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2h^2}{8ma^2}$$

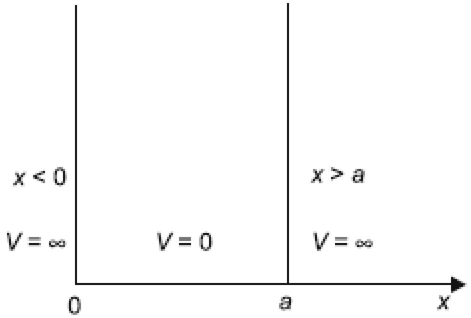


Fig. 1.7 One dimensional potential box

- Energies of particle in a one dimensional potential box are quantized and can be illustrated as in Fig. 1.8a.

- Corresponding wave functions and probabilities of different states of particle in the box would look like those in Fig. 1.8b, c

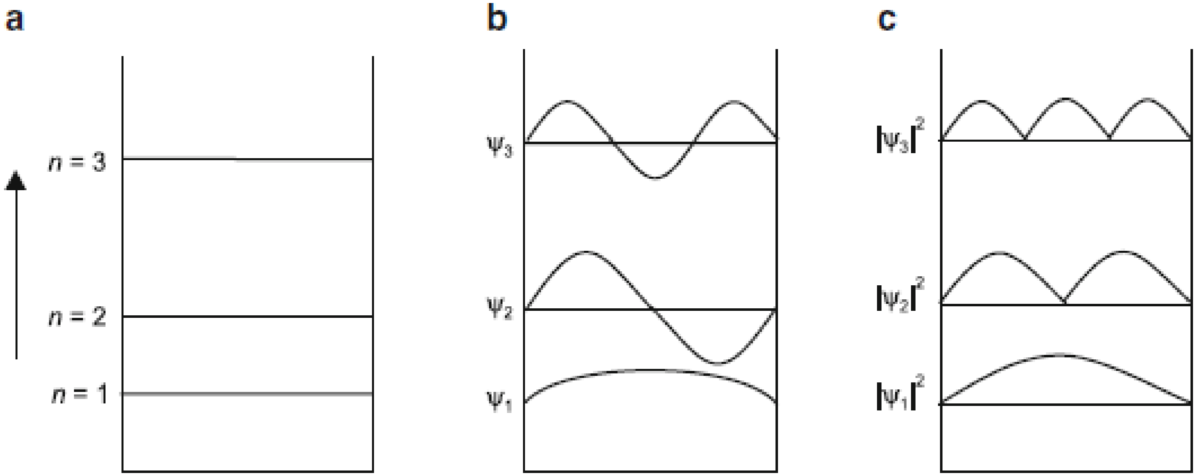


Fig. 1.8 (a) Quantized energy states, (b) corresponding wavefunctions and (c) probability of finding the particle at different locations between '0' and '*a*' in the box

1. Introduction to Quantum Mechanics

1.5.2 Density of State

Density of states *D(E)* is defined as the number of states per unit energy range

- Consider energy as is given for a particle in a 1D box

$$E_n = n^2 = \frac{h^2}{8ma^2} \quad \text{(Henceforth we drop suffix of } E\text{)}$$

$$dE = \frac{h^2}{8ma^2}.2n.dn$$

$$\boxed{\frac{dn}{dE}} = \frac{8ma^2}{h^2}.\frac{1}{2n} = \frac{a}{h}\sqrt{\frac{2m}{E}}$$

$$D(E) = \frac{dn}{dE} \propto E^{-1/2}$$

1. Introduction to Quantum Mechanics

1.5.2 Density of State

- Density of States for a Zero Dimensional (0D) Solid

A zero dimensional solid in which electron is confined in a three dimensional potential box with extremely small (<100 nm) length, breadth and height as a 0D solid

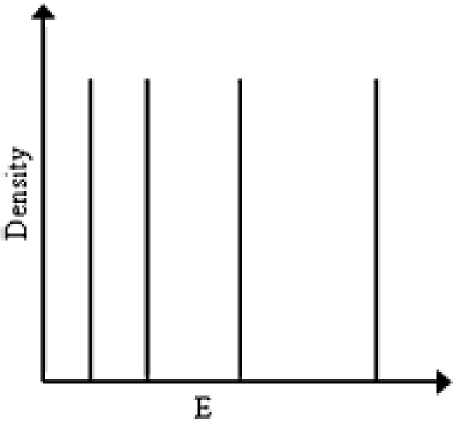


Fig. 1.9 Density of states for a particle in a zero dimensional solid

discrete energy levels as discussed above with density of states

$$D(E) = \frac{dN}{dE} = \sum_{\varepsilon_i} \delta\left(E - \varepsilon_i\right)$$

where ε_i are discrete energy levels and δ is Dirac function. The density of states as a function of energy would appear as illustrated in Fig. 1.9.

1. Introduction to Quantum Mechanics

1.5.2 Density of State

- Density of States in a One Dimensional (1D) Potential Box, Wire

A particle confined in one dimension is like a particle in a one dimensional potential well.

The potential in two directions is infinitely large but length is not very small

$$D(E) = \frac{dN}{dE} = \sum_{\varepsilon_i < E} \delta(E - \varepsilon_i)^{-1/2}$$

where ε_i are discrete energy levels. Figure 1.10 graphically illustrates nature of density of states for a one dimensional solid.

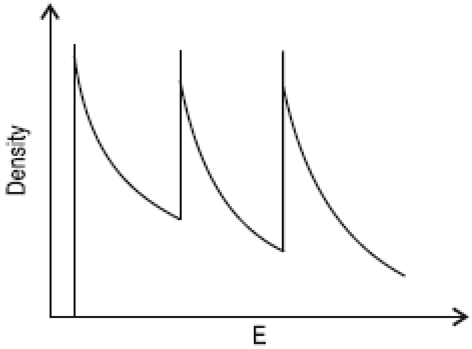


Fig. 1.10 Density of states for a particle in a one dimensional solid

1. Introduction to Quantum Mechanics

1.5.2 Density of State

- Density of States in a Two Dimensional (2D) Potential Box, Thin Film

$$D(E) = \frac{dN}{dE} = \sum_{\varepsilon_i < E} 1$$

the density of states in two dimensional case is constant

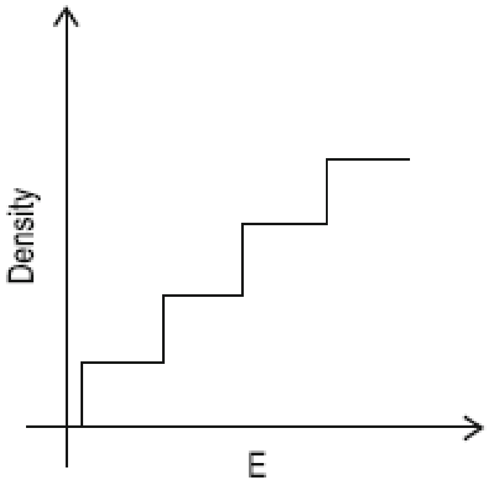


Fig. 1.11 Density of states for a 2D potential box

1. Introduction to Quantum Mechanics

1.5.2 Density of State

- Density of States for a Particle in a Three Dimensional Box (3D Bulk)

In a box of length ‘a’, width ‘b’, and height ‘c’ with potential $V = 0$ inside the box and V = ∞ outside the box, the energy states can be obtained as

$$E_{n_x,n_y,n_z} = \frac{\hbar^2}{2m}\left(n_x^2 + n_y^2 + n_z^2\right)$$

The wave function

$$\psi_n(x, y, z) = A\sin\left(\frac{\pi n_x x}{a}\right)\sin\left(\frac{\pi n_y y}{b}\right)\sin\left(\frac{\pi n_z z}{c}\right)$$

$$D(E) \propto E^{1/2}$$

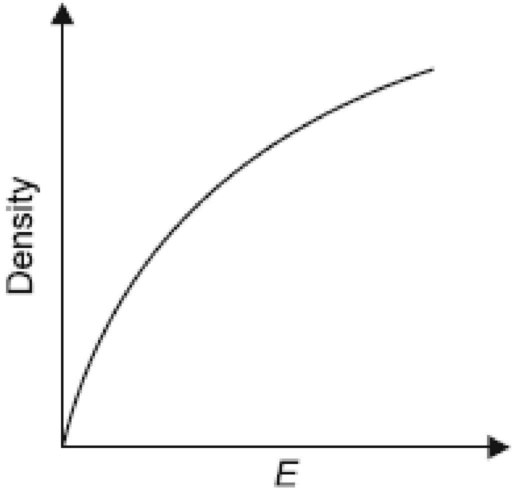


Fig. 1.11 Density of states for a 2D potential box

1. Introduction to Quantum Mechanics

1.5.3 Particle in a Coulomb Potential

- Another type of potential viz. Coulomb potential experienced by a particle

The potential can be written as $$V(r) = \frac{-Ze^2}{r}$$

negative sign means attraction between oppositely charged particles.

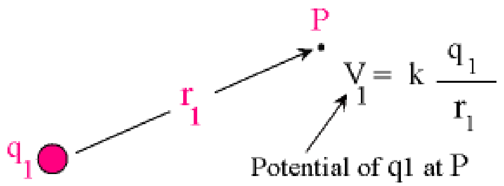
Where, '*Ze*' is the charge due to *Z* number of electrons and *r* is the distance between nucleus and the charge

<u>Electric Potential of a Point Charge:</u> (참고)

The electric potential V of a point charge q_1 at a typical point P in space at a distance r_1 from it is given by :

$$V_1 = k\frac{q_1}{r_1}$$

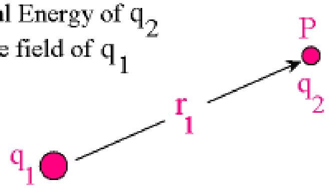
P is just a point in space.



Now if another charge like q_2 is placed at **P** a distance r_1 from q_1, then q_2 finds a potential energy equal to

$$\text{P.E.} = \frac{kq_1 q_2}{r_1} = V_1 q_2$$

Potential Energy of q_2 in the field of q_1

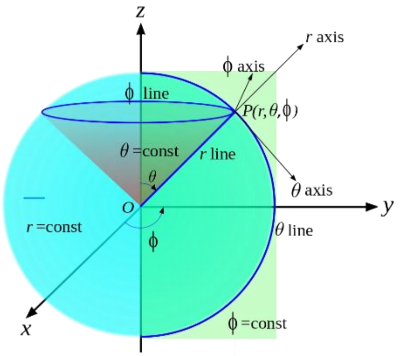


1. Introduction to Quantum Mechanics

1.5.3 Particle in a Coulomb Potential

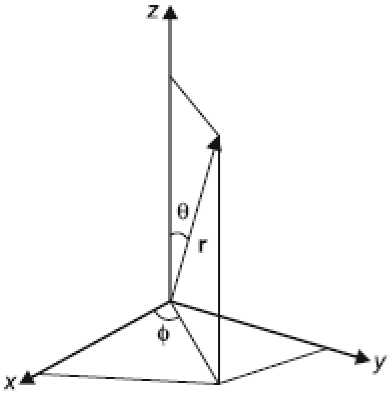
- When a particle moving in three dimensions is attracted towards the centre

  - For example an electron with negative charge attracted towards a positively charged nucleus at the centre of an atom.



Spherical coordinates

Cartesian coordinates by writing ψ, the wave function in spherical coordinates ψ (*r*, θ, φ).



$$x = r\sin\theta\ \cos\phi$$

$$y = r\sin\phi\ \sin\theta$$

$$z = r\cos\ \theta \text{ and } r = \sqrt{x^2 + y^2 + z^2}$$

The time independent Schrödinger equation in spherical coordinates can be written as

$$\nabla^2\psi(\mathbf{r},\theta,\phi) + \frac{2m}{\hbar^2}\left[E - V(\mathbf{r})\right]\psi(\mathbf{r},\theta,\phi) = 0$$

1. Introduction to Quantum Mechanics

1.5.3 Particle in a Coulomb Potential

- the spherically symmetric form of the potential

Wavefunction $\psi(r,\theta,\phi)$ is separable into functions of r, θ and φ as

$$\psi = R(r)Y(\theta,\varphi)$$

➡ $$\psi_{n\ell m}(r,\theta,\phi) = \frac{U_{n\ell}(r)}{r}Y_{\ell m}(\theta,\varphi)$$

$Y_{\ell m}$ are spherical functions

- The energy states can be obtained by considering one dimensional form

$$\nabla^2\psi(\mathbf{r},\theta,\phi) + \frac{2m}{\hbar^2}[E - V(\mathbf{r})]\psi(\mathbf{r},\theta,\phi) = 0 \longrightarrow \frac{-\hbar^2}{2m}\frac{d^2U}{dr^2} + \left[V(r) + \frac{\hbar^2}{2mr^2}\ell(\ell+1)\right]U = EU$$

Energy state of the system is described with three quantum numbers:

n (principal quantum number)
ℓ (orbital quantum number)
m (magnetic quantum number)

1. Introduction to Quantum Mechanics

1.5.3 Particle in a Coulomb Potential

- The angular momentum of the state is given by *L*

$$L^2 = \ell(\ell+1)\hbar^2 \quad \text{where} \quad \ell = 0, 1, 2, \dots (n-1)$$

- The <u>magnetic quantum number *m*</u> essentially gives component of angular momentum *L* parallel to *z* axis

$$L_z = m\hbar \quad \text{where} \quad m = 0, \pm 1, \pm 2, \cdots \pm \ell$$

The states are often denoted by *s*, *p*, *d*, *f* … to mean $\ell = 0, 1, 2$ etc.

- Consider now a Coulomb potential experienced by an electron of the form

$$V(r) = \frac{-Ze^2}{r}$$

where *Z* is atomic number, a situation in hydrogen atom (H), helium ion (He^+), lithium ion (Li^{2+})

Corresponding Schrödinger equation

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}\left(E + \frac{Ze^2}{r}\right)\psi = 0$$

1. Introduction to Quantum Mechanics

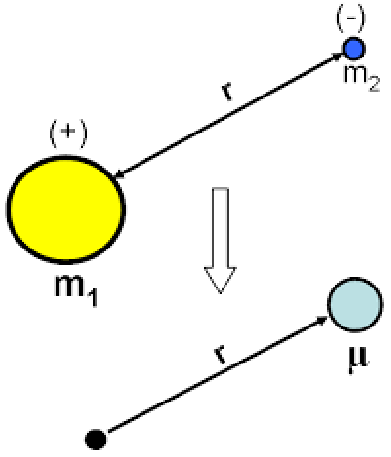
1.5.3 Particle in a Coulomb Potential

- The energy states by solving the equation in spherical coordinates

$$E_n = \frac{-2\pi^2 \mu Z^2 e^4}{n^2 h^2}$$

$$\frac{1}{\mu} = \frac{1}{m} + \frac{1}{M}$$

μ is called reduced mass that is mathematical description of motion in a vibrating or rotating two-body system (hydrogen)



$$n = \ell + 1, \ell + 2, \ell + 3 \ldots$$
$$\ell = 0, 1, 2, 3 \ldots (n - 1)$$

E_n is proportional to $1/n^2$, which means that energies will come closer as n increases

1. Introduction to Quantum Mechanics

1.6 Tunnelling of a Particle Through Potential Barrier

- A matter wave is incident on a potential barrier (from negative *x* direction)

Consider <u>one dimensional case</u>

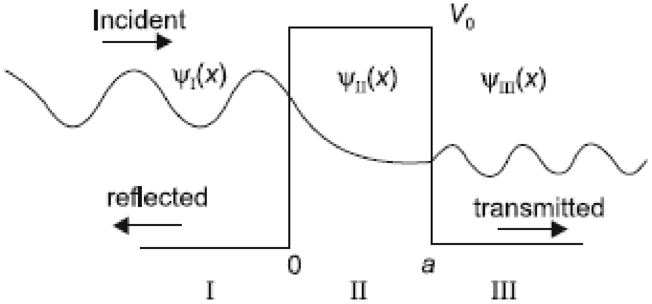


Fig. 1.13 Particle tunnelling through a potential barrier of height V_0. The kinetic energy of the particle is $E < V_0$. The particle is incident from left side in region I and by tunnelling through region II, escapes to region III with some probability of transmission, given by Eq. (1.73)

<Region I >

Energy of the particle is purely kinetic and potential $V = 0$

However, $E < V_0$ in region I, where V_0 is the potential at x=0

- Particle with less energy than the potential energy (V_0) as in region I,
- As long as V_0 is not infinite, There certainly exists a possibility that particle can not only <u>enter the region II</u> but also get <u>transmitted in region III and propagate</u>.

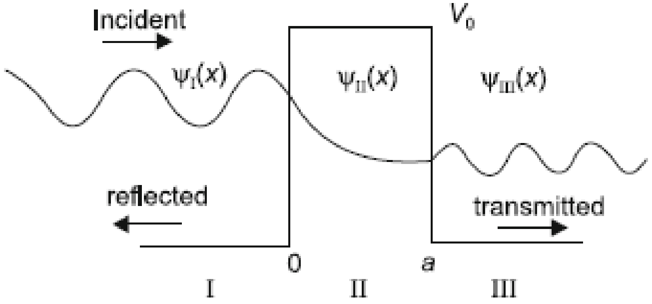
➡ 'Tunnelling of electron through insulating layer(dielectrics)'

1. Introduction to Quantum Mechanics

1.6 Tunnelling of a Particle Through Potential Barrier

- There is always a probability of <u>finding the particle on the other side of a potential barrier even though its kinetic energy is less than the potential barrier</u>

➡ Understanding many phenomena observed for subatomic particles and cannot be explained by classical mechanics



Reflection probability of wave in region I

$$R = \frac{{A_2}^2}{{A_1}^2} = 1 - T$$

- A particle with kinetic energy smaller than that required to overcome the potential energy of the barrier does have some probability of being on the other side of the barrier.

- This is quite important to explain quantum well structures, solid state lasers, light emitting diodes, particles inside the nucleus

Next

2. Structure and Bonding