# A First Course on Lasers and their Applications

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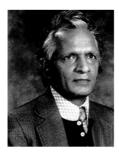
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To my academic mentors at the Indian Institute of Technology Kanpur, India, for continuous academic nurturing since July 1969, I joined the Ph.D. program in the Department of Physics.



Prof. Putch Venketaswarlu 1921-1997



Prof. Arvind Parasnis 1928-2011



Prof. Dasari Ramachandra Rao Thesis Supervisor 1932-2020

## TABLE OF CONTENTS

Prefacex
Introductionxiv
Chapter 1
<ul><li>1.6.4 Polarization</li><li>1.7 Electromagnetic spectrum</li></ul>
Chapter 2

2.1.5 Ultra-violet (UV) radiation generators
2.1.6 X-ray radiation generators
2.1.7 Gamma-ray ( $\gamma$ - ray) radiation generators
2.2 Amplification of IR-VIS-UV radiation
2.2.1 Gain in atoms and molecules
2.2.2 Stimulated emission in atoms and molecules
2.2.3 Population inversion techniques
2.3 Optical resonators
2.3.1 Stability criteria
2.3.2 Modes of a stable resonator
2.3.3 Unstable resonators
2.4 Generation of coherent IR-VIS-UV radiation
2.4.1 Resonator modes in the presence of a gain medium
2.4.2 Gain threshold and gain saturation
2.4.3 Anti-reflection coated and Brewster windows
2.4.4 Q-switching
2.4.5 Mode locking
2.4.6 Wavelength Tunability
2.5 Coherent emission from semiconductors in IR-VIS-UV regions
2.6 Coherent emission from free electrons in IR-VIS-UV regions
2.7 Harmonic generation in non-linear optical materials
2.8 Amplifiers in IR-VIS-UV region
2.9 Coherent emission in the X-ray region
Chapter 3
Coherent Generators and Amplifiers in IR-VIS-UV Regions
3.1 Introduction
3.2 Type-A lasers
$3.2.1 \text{ Cr}^{+3}$
$3.2.1.1 \text{ Cr}^{+3}$ : $Al_2O_3$ (ruby laser)
3.2.1.2 $Cr^{+3}$ : $BeAl_2O_4$ (alexandrite laser)
3.2.2 Nd <sup>+3</sup>
$3.2.3  Ti^{+3}$
3.2.4 Dye lasers
3.2.5 Rare gas ion laser
$3.2.6 N_2 laser$
3.3 Type-B lasers
3.3.1 He-Ne laser
3.3.2 CO <sub>2</sub> laser
3.3.3 He-Cd laser
3.3.4 Excimer lasers

3.4 Type C lasers	
3.4.1 Semiconductor junction lasers	
3.4.2 Free electron lasers	
Chapter 4	[
Application of Lasers in Basic Sciences	
4.1 Introduction	
4.2 Optogalvanic spectroscopy	
4.3 Doppler-free spectroscopy	
4.3.1 Saturation spectroscopy	
4.3.2 two-photon absorption	
4.4 Laser-induced breakdown spectroscopy LIBS	
4.5 Laser ablation	
4.6 Laser-heated pedestal growth of crystalline material	
4.7 Laser sintering	
4.8 Thermal conductivity measurement of insulators	
4.9 Radiation pressure	
4.10 Lasers in nuclear fusion	
4.11 Laser dosimetry	
Chapter 5	C
Commercial Applications of Lasers	
5.1 Introduction	
5.2 Holography	
5.3 Retail business	
5.4 Alignment of structures using lasers	
5.5 Laser material processing	
5.5.1 Hardening	
5.5.2 Drilling	
5.5.3 Cutting.	
5.5.4 Identification marks on components and products.	
5.5.5 Soldering and welding	
5.5.6 3D laser printer	
5.6 Lasers in health care	
5.6.1 Diagnostics	
5.6.2 Laser therapy	
5.6.3 Therapeutic surgery	
5.6.3.1 Laser cataract removal.	
5.6.3.2 Laser hemorrhoid surgery	
5.6.3.3 Laser removal of folliculitis	
5.6.3.4 Removal of internal stones	

- 5.6.3.5 Laser otology
- 5.6.3.6 Laser oral surgery
- 5.6.3.7 Laser brain surgery
- 5.5.3.8 Laser heart surgery
- 5.6.4 Laser cosmetic surgery
- 5.6.5 Manufacturing healthcare products
- 5.7 Laser agricultural weeding

#### **PREFACE**

The need for this Book, "A First Course on Lasers and Their Applications," emerged from my experience conducting about a dozen courses on lasers and their applications, primarily for the faculty members of engineering colleges in India. The motivation for these courses was to expose the faculty members to the field so that they could further train their students. Participants in these courses also included personnel from research laboratories who intended to initiate research in fabrication or applications in lasers; most of these participants were freshers who wanted to update their knowledge of lasers and their applications. Handouts were necessary due to the non-availability of a concise book fulfilling the requirements of these newcomers to the area. Such a book's deficiency was more while teaching BSc Physics Honorous students. The deficiency continues to the best of my knowledge.

A laser emits electromagnetic radiation like other sources, such as a filament lamp or a gas discharge tube. However, the properties of laser emission are orders of magnitude better than those of conventional sources. It is valid even when the emitting transition in an atom, ion, or molecule is precisely the same in a non-laser and laser emitter, implying that understanding electromagnetic emitting sources' mechanisms is fundamental to understanding laser emission. It requires detailed knowledge of the energy levels of the emitting materials. Exactly solving the relevant Schrodinger equation provides such information, which is often impossible. Data collected from experimental spectroscopy helps construct energy level diagrams, a graphical representation of energy levels of an atom, ion, or molecule. Labeling the energy levels in energy level diagrams is mostly in terms of quantum numbers; in some cases, labeling uses group theoretical nomenclature, confusing a beginner if not clarified adequately. Excitation and deexcitation processes in material result in the absorption and emission of radiation; transition from a lower energy level is absorption, while it is the other way around in emission. Material absorption needs an external energy source, while there are two emission modes: spontaneous and stimulated. Both have the same wavelength in case they originate from and terminate at the same energy levels. The former emission requires no external energy source, while the latter needs one, like absorption. The most xii Preface

dominant emission mode, the spontaneous emission, does not violate the thermodynamic population distribution in energy levels. If the stimulated emission mode dominates from the same material at the same wavelength, the material violates the thermodynamic-population distribution. How can we make it happen? Understanding matter-radiation interaction helps. Twelveth-grade-school level physics, chemistry, and mathematics are adequate for this understanding.

The same is the case with an understanding of optics used in lasers. It uses an optical resonator with a pair of mirrors or a mirror and a wavelength-tuning element adequately taught in 12th-grade school and first-year college. A beginner in lasers requires (i) enough quantum mechanics to understand the energy level structure of material emitting laser emission, (ii) enough optics to understand optical resonator and laser beam modification techniques, (iii) enough electrical and chemical engineering to understand techniques to make a material violate the thermodynamic principles and (iv) enough mechanical engineering to make the device mechanically stable. It is the guiding philosophy of this Book.

Laser application in basic sciences mainly includes applications with no non-laser option; if there is one, the accuracy increases by several orders of magnitude using lasers. Discussions on commercial applications of lasers point out the limitations of lasers.

Readers will find many intentional repetitions in this Book, intended to provide the necessary background to every new concept.

This Book, primarily for newcomers, provides to-the-point knowledge about the field. It includes the concepts adequately to understand lasers and their applications.

In one sentence, the Book is the first course on lasers and their applications recommended for newcomers in the field: students, researchers, and professionals.

I express my deepest gratitude to my spouse, Sheela, for her support, involvement, and endless patience while writing this Book. The motivation provided by regular conversations about the Book with my grandchildren Vihaan, Asmi, and Prithu is invaluable. Thanks to my children, Sheetu, Komal, Nishant, and Shirish, for standing by me. I am grateful to Dr. Jasiya Mushtaq Al-Azhariya, an Arabic Scholar from Kashmir, for her encouragement and keeping my spirits up by sharing Kashmiri music. The

help and concern of my MSc (Physics) student at IIT Kanpur, Mr. Anil Singal, is gratefully acknowledged.

The cooperation and patience of Mr. Vijay Ganpatrao Kadam, who prepared most of the line diagrams for the manuscript, are gratefully acknowledged.

Finally, thanks to Cambridge Scholars Team Members for their patience and efforts in publishing this Book.

Bansi Lal Pune, India

#### **INTRODUCTION**

The introduction briefly outlines the main content of each Chapter of this Book; it has five chapters. Chapter 1, titled "Matter and Electromagnetic Radiation," describes the UV catastrophe that led Planck intuitively to the concept of the "light energy packet," the photon. Plankck's law explains the observed properties of thermal radiation, eliminating the existence of UV catastrophe. This path-breaking concept led to the development of quantum mechanics. The Chapter describes the preliminary quantum concepts necessary to understand lasing mechanisms, particularly the properties of the energy level structures of atoms, ions, and molecules gain media for laser emission. The Chapter ends by introducing the concept of stimulated emission of radiation to derive Planck's law from matter-radiation interaction.

The title of Chapter 2 is "Generation and Amplification of EM Radiation." It discusses the generation of incoherent radiation from radiowaves to cosmic rays. It also explores the possibility of coherent emissions in each region. The Chapter details the mechanism and technology of coherent emission in IR-VIS-UV, infrared-visible-ultraviolet regions. Discussion includes population inversion techniques, stable and unstable optical resonators, Q-switching, mode-locking, and wavelength tuning. The Chapter discusses coherent emission from atoms, molecules, ions, semiconductors, and free electrons. It includes a discussion on amplifier chains.

Chapter 3, "Coherent Generators and Amplifiers in IR-VIS-UV Regions," discusses the commercially viable lasers in IR-VIS-UV regions categorized as Type A, B, and C. The gain produced in the gain media of Type A lasers is due to its inherent energy level structure; a suitable pumping technique produces the gain. In the case of Type B, the gain in material X requires Y or more media to achieve it. In type C, the stimulated formalism is not applicable straightforwardly. The number density and radiation field build-up result in coherent emission; coherent emission from semiconductors and free electrons are the two examples

"Application of Lasers in Basic Sciences," title of Chapter 4, discusses the application of lasers in research and development in physics, chemistry, biology, geology, etc. It discusses advanced spectroscopic techniques like optogalvanic spectroscopy, Doppler-free saturation, and two-photon

absorption spectroscopy. The Chapter also discusses methods like laser-induced breakdown spectroscopy, thermal conductivity measurements of insulators, laser ablation and its near-future commercial applications, laser sintering, investigations on radiation pressure, and laser cooling and its applications. It also includes a discussion on laser fusion.

The title of the last Chapter, Chapter 5, is "Commercial Applications of Lasers." It discusses the underlying principle of machines using lasers for various commercial applications; without naming the model numbers or manufacturers, The Chapter discusses holography and its commercial applications, lasers in the retail business, industrial alignment, 3D printing, health care, and agricultural weeding, Health care section discusses the applications in diagnostics and surgery; surgery includes both therapeutical and cosmetic procedures.

#### CHAPTER 1

### MATTER AND ELECTROMAGNETIC RADIATION



Fig 1-1 Typical items used to start a new day

#### 1.1 Introduction

Most people start their day with tea or coffee and electronic devices like phones and smart speakers; Fig 1-1 shows such typical items like a kettle, a cup, a phone, a smart speaker, a power extension board, and connecting wires, classified as matter that has a mass and occupies some physical space called volume. The state of motion of a body (a piece of matter) determines its mass. If a body is at rest in its surroundings, its mass, termed rest mass, is an invariant quantity. Matter has five states: solid, liquid, gas, plasma, and Bose-Einstein condensate (BEC). These states are interchangeable by temperature manipulation. Water, for example, is solid (ice) at a temperature of  $T \le 0$  °C. It is liquid (water) in the temperature range of 0-100 °C, while gas (steam) for T >100 °C. About 3% of water molecules (H<sub>2</sub>O) dissociate into atomic hydrogen (H) and oxygen (O) when heated to around 2200 °C. H splits into a hydrogen ion (H<sup>+</sup>) and an electron at about 9726 °C. This electron removal from an atom is ionization. The amount of external energy required to ionize an atom is its ionization energy. A thermal source is one of many external energy sources that ionize an atom; it is thermal ionization. The thermal ionization of H starts at about 6700 °C, while above 9700 °C, most of it is ionized. An ensemble of hydrogen atoms heated to 9700 °C or more consists of H<sup>+</sup> ions, electrons (e), and neutral hydrogen atoms; H<sup>+</sup> and e are the free charge carriers of such an ensemble. The number of free charge carriers per unit volume of the ensemble is its density. Its magnitude affects the physical properties of such an ensemble. At a particular critical density, the ensemble shows collective behavior;

such an ensemble is thermal plasma. There are other techniques to produce plasma; a description of those techniques is beyond the scope of this Book. Similarly, at temperatures close to 0 K, an ensemble of particles under suitable conditions exhibits collective properties; such an ensemble is Bose-Einstein condensate.

The electric power provided to the kettle and the smart speaker cannot be classified as matter because they have zero rest mass and do not occupy any physical space. The same is valid with the Wi-Fi signal fed to the phone and the speaker. However, both are some forms of energy. The electric power in the form of electric current propagates in a medium (electric conductor). On the other hand, Wi-Fi is electromagnetic energy, termed electromagnetic radiation (EMR). It propagates in free space with a velocity of c (~3.0 x 10<sup>8</sup> m/s); c is a universal constant. It can propagate through various materials with velocity v, which numerically differs from c; v is a characteristic of the material that propagates EMR. When heated, matter emits EMR, also called thermal radiation (TR). The remaining sections of this Chapter discuss the laws and the mechanism of producing TR and its interaction with matter. It also includes the relevant portions of quantum mechanics and the electronic structure of matter to understand the mechanism of the TR sources and TR-matter interaction.

### 1.2 Thermal radiation (TR)

All matter at temperature T > 0 K emits thermal radiation. The sun is an interesting TR emitter. It is an essential energy source for life on Earth. Fig 1-2 shows a typical spectrum of sunlight recorded by a spectrograph designed for the radiation in the wavelength range 400-700 nm (1 nm equals  $10^{-9}$  m). As seen in this figure, the radiation from the sun is composed of bands of violet, blue, green, yellow, and red colors without any sharp boundaries between them. This type of spectrum is known as a continuum or band spectrum. An average human eye can perceive the wavelength region from 400 to 700 nm. Hence, it is the visible region; many heavenly bodies like stars also emit in it.

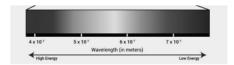


Fig 1-2 Visible Spectrum of the sunlight recorded on a spectrograph; Reference UV-Visible Spectroscopy (msu.edu)

#### 1.2.1 Ultraviolet catastrophe

Matter like iron shows interesting emission properties with the change in its temperature, as seen in Fig 1-3, where a heat source like an oxyacetylene flame continuously heats the tip of an iron rod.



Fig 1-3 Colours perceived by a normal human eye from a heated iron piece; reference The Definition of Conduction in Physics (thoughtco.com)

Heat conduction through the rod increases the temperature of its various parts, while radiation from the rod surfaces is a loss mechanism; the equilibrium between the two determines the net temperature rise at a particular point. There is a temperature gradient from Region 1 to 3; the highest temperature is in Area 1, while the lowest is in Region 3. Region 1 looks white when its temperature is about 1200 °C while Area 2 looks red at about 900 °C. Area 3 looks grey at about 25 °C. This simple demonstration implies that the color of the emission from iron depends on its temperature; hence, the emission is TR. Fig. 1-4 shows the spectrum of this emission (white light) from Region 1 recorded on a standard spectrograph; it is the TR spectrum of iron in the visible region 400 to 700 nm.



Fig 1-4 Typical thermal emission (TR) spectrum of a heated Fe, reference iron spectrum (nist.gov)

As stated earlier, the wavelengths of the spectra in Figs 1-3 and 1-4 are in the 400-700 nm (visible) region; however, unlike the solar spectrum, the

iron emission spectrum has well-spaced lines. These lines are the images of the slit of the recording spectrograph, and such spectrum is a line spectrum. Emission spectra, both line and band, are characteristic of the emitter; hence, the diagnostic tools to identify the emitting material.

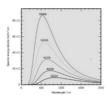


Fig 1-5 Variation of the intensity of the emitted radiation as a function of its wavelength, reference Thermal radiation - Wikipedia

Fig 1-5 plots the measured thermal emission energy density (spectral energy density in kJ/m³-nm) as a function of the emitted emission wavelength (nm); each curve in this figure represents an emission profile at a particular temperature of the emitting material. The overall shape of each curve in this figure is identical: a rise in intensity with the increase in wavelength, peaking at a particular wavelength followed by a continuous decrease at higher wavelengths. The peak ( $\lambda_{peak}$ ) of the emission profiles (Fig 1-5) shifts towards the shorter wavelengths, red to blue, with the increase in the emitter temperature. Wien's displacement law explains this observed shift in  $\lambda_{peak}$ . Wein, using thermodynamic arguments, derived this law in 1893. It states that the  $\lambda_{peak}$  is inversely proportional to the temperature T of the emitter. Mathematically

$$\lambda_{peak} = b/T \tag{1.1}$$

b is Wien's constant.

The area under the emission profile (Fig 1-5) is the total thermal power P (W) across all the wavelengths emitted by the emitter at a particular temperature. Stefan-Boltzmann's law relates the P (W) from a heated emitter to its temperature T K. Mathematically.

$$P(W) = A\varepsilon\sigma T^4 \tag{1.2}$$

A  $(m^2)$  is the emitter's surface area, and the proportionality constant  $\sigma$  is the Stefan-Boltzmann constant.

The emissivity  $\varepsilon$ , is the measure of the emitting properties of the emitter surface. Its value for a perfectly emitting surface is one; such a surface, the black body, is an ideal emitter. The emissivity is less than one for all the practical emitters and generally has a wavelength dependence.

Rayleigh-Jeans law is the first wavelength ( $\lambda$ )-dependent expression for the power emitted by an emitter heated to temperature T K. Derived using the concepts of the equipartition energy theorem of classical mechanics, the mathematical form of the law follows.

$$B_{\lambda}(T) = 2ckT/\lambda^4 \tag{1.3a}$$

 $B_{\lambda}(T)$  is the radiation density, the amount of power radiated per unit emitted area, wavelength, and solid angle; c is the velocity of light in vacuum; and k is the Boltzmann constant. Eq 1.3b expresses frequency (v) dependent radiation density  $B\nu$  (T).

$$B_{v}(T) = 2kTv^{4}/c^{3}$$
 (1.3b)

There is no time dependence in Eq 1.3a and Eq 1.3b, implying that these equations apply to the emitters at thermodynamic equilibrium.

Equation 1.3a could not reproduce the experimentally observed emission profile shown in Fig 1-5. This equation predicts that spectral radiance increases rapidly with the decrease in wavelength. It is almost infinite at low wavelengths, contradicting the observed emission profile shown in Fig 1-5. This breakdown of the classical interpretation of the thermal sources at short wavelengths is known as the ultraviolet catastrophe.

#### 1.2.2 Planck's radiation law

Rayleigh-Jeans derived Eq 1.3a, assuming that the average energy kT is a continuous function of the temperature, which also changes continuously. It can take continual values with the temperature change, irrespective of the wavelength (frequency) of the emitted radiation. Planck modified it intuitively. He assumed that any change in temperature results in an increase or decrease of energy only by an amount  $\Delta E$  proportional ( $\infty$ ) to the frequency (wavelength) of the emitted radiation. Mathematically

$$\Delta E \propto v \text{ or } \Delta E = hv = hc/\lambda$$
 (1.4)

Where h is Planck's constant, Eq 1.4 implies that the energy of TR changes only in packets (quantum) of magnitude hv ( $hc/\lambda$ ) with temperature. It is composed of quanta, plural for the term quantum. The expression derived by Planck for the density of the radiation emitted by a thermal source in thermodynamic equilibrium in the wavelength domain is:

$$B_{\lambda}(T) = 2hc^{2}/\lambda^{5} \left[ 1/(e^{hc/\lambda kT}-1)^{-1}) \right]$$
 (1.5)

Eq 1.5 in the frequency domain looks like

$$B_{\nu}(T) = 2h^{2} \nu^{3} / c^{2} [(e^{h\nu/kT} - 1)^{-1}]$$
(1.6)

Eq 1.5 is like Eq 1.3a except for the exponential factor  $[1/(e^{hc/\lambda kT}-1)^{-1}]$ , which results from the assumption that energy can take only discrete values depending on the wavelength. It is the quantization of energy.

The denominator of Eq 1.5 has two terms, (i)  $\lambda^5$  and (ii) the exponential  $(e^{hc/\lambda\,kT}-1)$ . Term (i) approaches zero with the decreasing wavelength, while term (ii) approaches  $e^\infty=\infty$ . The product of term (i) and term (ii) tends to  $\infty$  when wavelength decreases, so Eq 1.5 tends to zero, eliminating the ultraviolet catastrophe predicted by Rayleigh-Jeans' law (Eq 1.3a). Planck's law (Eq 1.5 and Eq 1.6) faithfully reproduces Fig 1-5 and initiates quantum physics.

The standard technique to find the maxima of the distribution represented by Eq 1.5 is (i) to calculate the differential of Eq 1.5 with  $\lambda$  and (ii) equate the result to zero. Mathematically

$$d[B_{\lambda}(T)] / d\lambda = 0 \tag{1.7}$$

After solving Eq. 1.7, one obtains:

$$T \lambda_{\text{max}} = \text{hc/5k} \tag{1.8}$$

Eq 1.8 is identical to Eq 1.1, Wien's displacement law.

The exponential  $e^{hc/\lambda kT}$  decreases with the increase in  $\lambda$ ; at a sufficiently high value of  $\lambda$  it can be approximately written as  $1+hc/\lambda kT$  so that the Eq 1.5 takes the following form:

$$B_{\lambda}(T) = 2ckT/\lambda^4 \tag{1.9}$$

Eq 1.9 is identical to Eq 1.3a, implying that Planck's law at higher wavelengths takes the form of Rayleigh-Jeans law, which successfully explains the higher wavelength side of Fig 1-5.

As mentioned earlier, Planck intuitively introduced the concept of energy quanta; the subsequent work by many people proved its existence. It led to the development of a new theory of matter and radiation called quantum physics. The following sections discuss the portions of this theory relevant to the understanding of this Book.

#### 1.3 Quantum Physics

The main features of quantum physics are:

- (i) The magnitude of physical quantities is quantized; values are discreet, not continuous, as in classical physics.
- (ii) Minimum uncertainty is inherent in all measurements.
- (iii) Wave-particle duality,
- (iv) Entanglement

All the above four features are, in principle, applicable to all matter irrespective of its size; however, all these effects can be observed only at a microscopic scale in the case of atoms and sub-atomic particles.

#### 1.3.1 Quantization

Quantization means that physical quantities like linear and angular momentum, energy, charge, etc., take only discrete values; all values are the characteristic smallest value multiplied by integers 1, 2, 3, etc. The smallest value is a quantum, while the integers are quantum numbers. The structure of a typical atom elucidates the concept of quantization. Negatively charged electrons e, positively charged protons p, and electrically neutral neutrons n are the primary constituents of an atom. The number of e, p, and n is always an integer; quantum one is multiplied by 1,2,3, and so on. Hence, 1 is the quanta for the particle number present in an atom. An electrically neutral atom has the same number of electrons and protons. This number is called the atomic number. The negatively charged electron has a charge of about  $1.6 \times 10^{-16}$  C, while its mass is about  $1.1093 \times 10^{-31}$  kg. On the other hand, a proton and a neutron have almost the same mass, about 1800 times heavier than an electron.

Protons and neutrons form an atom's central core, the nucleus. The electrons move in quantized orbits around the core. The quantized physical properties associated with the orbital motion of the electrons are momentum and spin. These quantized orbits are called stationary orbits, where the electrons do not radiate even when continuously in an accelerated state of motion, a clear violation of classical electrodynamics.

The orbital angular momentum L of an electron is

$$L=h/2\pi \left[l(l+1)^{1/2}\right]$$
 (1.10)

l is the angular momentum quantum number, and l = 0,1,2,3,4, etc. Since an electron also spins, a spin angular momentum  $S = h/2\pi$  [m(m+1]<sup>1/2</sup>; m = 0,1,2, 3, etc. L and S are vectors; when added vectorially, total angular momentum L+S=  $J = h/2\pi$  [j(j+1]<sup>1/2</sup>; j= 0, 1, 2, 3, etc.

Quantized energy  $(E_2-E_1) = hv$  is emitted or absorbed by the atom whenever one or more electrons change the orbit. This inter-orbital transfer of electrons involves the change in quantum numbers. Hence, well-defined selection rules govern the transfer. Any discussion about these selection rules is beyond the scope of this Book.

#### 1.3.2 Heisenberg uncertainty

In classical physics, the magnitude of a physical quantity is, in principle, measured with zero inaccuracy. Any inaccuracy is mainly due to the measuring tools; improving their quality minimizes measurement inaccuracy. Classical physics does not limit the achievable accuracy of any measurement. If  $\Delta x$  denotes the inaccuracy in the position measurement of a moving body and  $\Delta p$  that of its momentum, classically, in the case of a simultaneous measurement, the product  $(\Delta x \ \Delta p)$  tends to zero with the improvement in the measuring techniques. On the other hand, quantum physics postulates an inherent inaccuracy, the Heisenberg uncertainty; it limits the accuracy of the simultaneous measurement of  $\Delta x$  and  $\Delta p$ , a conjugate pair. Any improvement in measuring instrumentation cannot correct the Heisenberg uncertainty. The product  $(\Delta x \ \Delta p)$  has a minimum value given by:

$$(\Delta x \, \Delta p) \ge h/4\pi \tag{1.11}$$

The other conjugate pair is time (t) and energy (E), where we have:

$$(\Delta t \Delta E) \ge h/4\pi \tag{1.12}$$

The numerical value of Planck's constant h is 6.626 x 10<sup>-34</sup> J.s; hence, Eq 1.11 and Eq 1.12 are relevant in subatomic physics.

#### 1.3.3 Wave-particle duality

Classical physics clearly distinguishes a particle from a wave. Three-position coordinates x, y, and z specify the location of a particle in a three-dimensional space at a time t. Momentum p (product of mass and velocity) reflects its state of motion. On the other hand, a wave is a propagating disturbance that may or may not need a physical medium for propagation. Such is not the case in quantum physics, where a classical particle may behave like a wave in a particular situation and vice versa. Quantum physics describes a physical system in terms of a wave function  $\Psi$ . It may act as a classical particle in a specific application and a classical wave in a different situation. This situation-dependent behavior is wave-particle duality. To elucidate it further, let us understand the working of a photomultiplier tube (PMT) widely used to analyze the radiation in the visible region. Fig 1-6 shows the schematics of a typical PMT tube.

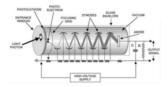


Fig 1-6 Schematics of a typical photomultiplier tube, reference Photomultiplier Tubes (PMT) (sense-pro.org)

Visible radiation (light photon) falls on the photocathode of a PMT, as shown in Figs 1-6; the photocathode must be compatible with the frequency of the radiation to detect. This radiation results in the emission of electrons, known as photoelectrons. These photoelectrons hit the first dynode of the PMT, where the number of electrons gets amplified due to secondary electron emission. Dynode 2 further increases the number of secondary electrons emitted from Dynode 1. The process continues with many more dynodes to get the measurable electron current required for detection. The particle nature of the electrons is responsible for the secondary electron emission. To eject an electron from metal, the minimum kinetic energy  $KE_{\rm e}$  is given by:

$$KE_{e} = e\phi \tag{1.13}$$

e is the electron charge. Work-function  $\phi$ , is the characteristic property of the material used for electron emission. Eq 1.13 sets a threshold for the kinetic energy of the incident electrons. If  $KE_e < e \phi$  secondary emission is not possible,  $KE_e \ge e \phi$  results in the secondary emission. On the other hand, assuming the wave nature of visible radiation, the threshold condition  $KE_e \ge e \phi$  may be satisfied near the peak of the radiation wave. If it is true, there will be an observable delay between the incidence of the radiation and the observation of the emitted electrons. No such delay is observable experimentally, making it imperative to assume the particle nature of the radiation. Historically, Einstein explained the emission of electrons by radiation, known as the photoelectric effect, in terms of photons, the particles of radiation. Photons have zero rest mass. Its energy E = h v; v is the frequency, and h is Planck's constant. The necessary condition to observe the electron emission by a photon is  $hv \ge e \phi$ . The photoelectric effect sets the 'wave-particle' ball rolling.

Next, examine if the classical particle electron can show wave-like properties. The most straightforward test to ascertain the wave nature of the electrons is to investigate if the electrons diffract like photons. Fig 1-7 shows a typical experimental setup to investigate electron diffraction.

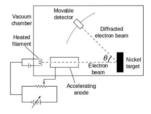


Fig 1-7 Typical experimental setup to investigate electron diffraction, reference File: Davisson-Germer experiment edit1.svg - Wikipedia

The experimental arrangement resembles the single-slit setup described in the introductory optics textbooks. A detector on a variable platform records the electrons after an electron beam interacts with a Ni target. If the electrons do not have any wave-like nature, the detector output will be just the central white spot of Fig 1-8. However, the concentric rings of decreasing intensity as one moves away from the point of maximum output are the typical characteristics of a diffraction pattern. This observation confirms the wave nature of the electrons.



Fig 1-8 Typical detector output confirming the wave nature of the electrons.

#### 1.3.4 Entanglement

Imagine a pair of design-wear shoes. One can have almost complete information about the other shoe thousands of *miles* away by looking at one shoe of the pair. If the wearers have the shoe for the left foot, they are sure the other shoe would fit their right foot whenever found. It is entanglement. The pair shares information about each other irrespective of their physical distance. Similarly, two or more particles are entangled when a single quantum state characterizes the particle ensemble. Quantum computers use quantum entanglement for faster calculations compared to classical electronic computers.

#### 1.4 Electronic structure of matter

All matter is composed of atoms. As stated, the atoms have a core part, the nucleus, constituting positively charged protons and neutral neutrons; negatively charged electrons move in well-defined orbits around the nucleus. Quantum mechanics describes the motion of electrons around the nucleus in terms of wavefunctions and quantized energy levels. Besides atoms, there are ions and molecules. An ion has more or fewer electrons than its parent atom. If the number is more, it is a negative ion; otherwise, it is a positive if the number is less. Removal of electrons from an atom results in the formation of positive ions, while the creation of negative ions needs the addition of electrons to an atom.

On the other hand, the sharing of electrons between two or more atoms forms molecules. The following sections discuss the introductory electronic structure of atoms, ions, and molecules essential to understanding the subject matter of this Book.

#### 1.4.1 Atoms and ions

Let us start with the first element in the Periodic Table, the hydrogen atom, H, which has a proton p as its nucleus and one orbital electron e, as shown in Fig 1-9

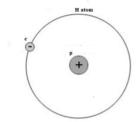


Fig 1-9 Pictorial description of a hydrogen atom

The general expressions for the radius  $r_n$  and the energy  $E_n$  of the electron are:

$$r_n = (0.529 \times 10^{-10} \text{ n}^2) \text{ m}.$$
 (1.14)

$$E_n = (-13.6 / n^2) \text{ ev}$$
 (1.15)

The principal quantum number is n in Eq 1.14 and Eq 1.15. Its values are 1,2, 3, and so on; it cannot be zero or negative. Electron volt (ev) is the unit of energy;  $1 \text{ ev} = 1.602 \text{ x} 10^{-19} \text{ J}$ .

When n=1,  $E_n=$  (-13.6ev). The energy is negative because the orbital electron is bound to the nucleus due to electrostatic attraction. The minimum energy required to free the electron from the attractive force of the nucleus is 13.6 ev; it is also called binding energy. The orbit with n=1 in the H atom has one electron and a population. No electrons exist in orbits with n=2, 3,4,5; the orbits with n>1 are unpopulated.

The magnitude of the positive charge of the nuclear proton is precisely equal to the negative charge on the orbital electron, making the H atom electrically neutral. However, upon removing the electron entirely from the influence of the nuclear electrostatic field, the resulting atom will no longer be electrically neutral; it will have a positive charge because of the proton in the nucleus. The symbol for such an atom is H<sup>+</sup> (positive hydrogen ion). As stated earlier, the conversion of H into H<sup>+</sup> is the ionization process, and the amount of external work required to ionize it is its ionization potential,

which is 13.6 ev. On the other hand, H can change to H<sup>-</sup> (negative hydrogen ion) by adding one more electron.

Fig 1-10 is an alternate pictorial representation of the electronic orbits of an H atom. It is an energy level diagram where the principal quantum number n designates the energy levels; a set of quantum numbers generally classify each in a more detailed diagram.

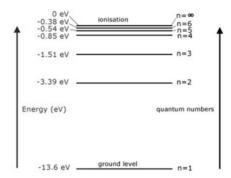


Fig 1-10 Pictorial representation of the allowed quantized orbits of an electron in an H atom. This representation is called the energy level diagram, reference Electricity - detailed contents (a-levelphysicstutor.com)

In Fig 1-10, the energy level  $E_1$  corresponding to n=1 is the ground level. This energy level is populated at standard temperature and pressure, while all other levels correspond to n=2,3,4, n.( corresponding energies are  $E_2$ ,  $E_3$ ,  $E_4$ ..... $E_n$ ) are unpopulated. Energy equal to  $(E_2$ - $E_1)=10.21\,\mathrm{ev}$ , supplied externally, can induce the electron transfer from  $E_1$  to  $E_2$ . It is an electronic transition; the term applies to both the transfers from a lower energy level to a higher energy level and vice versa. A transition does not take place arbitrarily. There are well-established selection rules; the relevant sections discuss these rules.

An electron populating the ground energy level can stay forever unless forced to move to a higher energy level by an external energy source; its lifetime in the  $E_1$  is infinite. A ground energy level at standard temperature and pressure always has a population. Transferring the electrons from the ground energy level to a higher level does not happen without an external energy source. It is not a spontaneous electronic transition; it is induced or stimulated; energy from an external source provides the stimulation. On the other hand, electrons in higher excited energy levels,  $E_2$ ,  $E_3$ ,  $E_4$ , etc., can decay to the ground or lower energy level without any external energy; in

such cases, the decay is spontaneous. The spontaneous decay mode is the most dominating. However, there is a possibility of stimulated decay, which is responsible for the existence of coherent emitting sources, the subject matter of this Book

Unlike the ground energy level, an excited one has a finite lifetime. It is the average time an electron stays in the energy level. The observed lifetime varies from nanoseconds to tens of seconds; a few exceptional systems have lifetimes of the order of femtoseconds.

As stated earlier, transitioning from a lower to a higher energy level requires external energy. In comparison, a transition from a higher to a lower energy level results in the release of energy. The transition where the energy is released as EMR is a radiative transition; otherwise, it is non-radiative. Population at a higher energy level can decay partly radiatively and partly non-radiatively. The radiative transitions among the electronic levels generate most of the radiation emitted by celestial bodies like stars and artificial radiation sources.

 $\Psi_n$  is the wave function of an energy level in Schrodinger terminology; n is the principal quantum number of the energy level. Alternately, the Dirac formalism uses bra (<) and ket (>) notation; n> is equivalent to  $\Psi_n$ . Another relevant term is the transition probability  $P_{ij}$ . It measures the probability that an electron in level i ( energy  $E_i$  ) will likely transit to another level j ( energy  $E_j$ ). Mathematically

$$P_{ij} = [\langle n_i | H_{ij} | n_j \rangle]^2 \tag{1.16}$$

The interaction Hamiltonian  $H_{ij}$  is electric, magnetic, or a combination of both.

If  $< n_i \mid H_{ij} \mid n_j > \neq 0$ , the transition between the energy levels i and j is allowed;  $H_{ij}$  couples the two energy levels. It is not the case when  $< n_i \mid H_{ij} \mid n_f > = 0$ . However, interactions other than particular  $H_{ij}$  may couple the two. Electric interaction, for example, may not allow a specific electronic transition, but magnetic interaction may enable it.

By computing Eq 1.16, information about the allowability of transitions, transition probabilities, and decay times is obtainable. The technique has worked well for hydrogen-like systems with only one orbital electron. However, it is difficult for systems with more than one orbital electron. Empirical energy level diagrams obtained from spectroscopic data for