

Module 1: History of Atomic & Molecular Physics and basic backgrounds

Lecture – 1

TITLE: Introduction to Atomic and Molecular Physics

Objectives

Atomic and molecular physics is an interesting and important subject to understand and invent the world.

Here, we start with a brief introduction of atomic and molecular physics.

The overview of different area of basic research in this field is discussed.

The develop methodology for understanding the insight of many other fields of research is described.

The concepts developed in this field which helped to realise many devices for medical and household applications are outlined.

Introduction

- The Atomic and Molecular Physics is the world of Atoms, Molecules, Ions, Clusters and Photons.
- It is the one of the most fundamental and important field in development of knowledge in Physical and Chemical sciences.
- It is the oldest branch of Quantum Physics. The field contributed so much to the development of quantum mechanics that until thirties of last century, atomic and molecular physics was inseparable from quantum physics.
- It remains one of the most important subjects for the testing grounds of the quantum theory.
- In spite of being the oldest field, it has retained its freshness all along and is continuing to contribute to the understanding of the fundamental laws of nature and also to the development of new technologies.

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Research in this area today encompasses the study of structure and interaction of atoms, molecules, ions, biomolecules, clusters at wide ranging scales.

- Providing newer insights into practically all field of science and technology, such as:
Spectroscopy, Laser Physics & Technology, Plasma Physics, Nuclear physics, Non-accelerator Particle Physics, Astrophysics, Condensed Matter Physics and Material Sciences, Metrology, Biosciences, Atmospheric Sciences.

Chemical sciences mainly analysis and reactions, biological physics, energy research and fusion studies.

Varieties of applications:

Laser, X-ray technology, Nuclear Magnetic Resonance (NMR), Magnetic Resonance Imaging (MRI), Electron Paramagnetic Resonance (EPR), Mossbaur spectroscopy, Laser atom cooling, Bose Einstein Condensation (BEC), GPS system for navigation, Pollution detection, Various medical applications etc.

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- Wide ranging scales make the field of Atomic & Molecular Physics more interesting today than it was ever.
- We also see that the study of atomic and molecular physics is at the heart of every interdisciplinary research.
- An understanding of the structure of atoms and molecules is therefore a prerequisite for entering into several of the areas discussed earlier.

Various scales in Atomic Molecular Physics:

In the following, we will come to know the characteristics of the atoms and molecules in various conditions in terms of temperature, photon intensities and frequencies.

(Temperature range from $10^4 K$ to $10^{-9} K$)

$\sim 10^4 K$

Fusion Plasma and stellar environment, Spectroscopy and dynamics of highly charged ions, Diagnostic techniques for plasma

$\sim 10 K$

Molecular interactions in astrophysical ices, Formation of complex molecules in interstellar environment, Fundamental question on formation of molecules which have relevance to origin of life

$\sim 10^{-1} K$

Atomic and Molecular beams, Clusters

$\sim 10^{-6} K$

Laser cooled atoms, Atomic clock based on Cs fountain, Nano-fabrication using cold atoms,

$\sim 10^{-9} K$

Quantum degenerate atomic gases, Bose-Einstein Condensation, Fermi Sea, Quantum many body physics, Matter wave optics, Atom interferometry, Atomic Physics as basis of condensed matter physics

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Photon intensities used for interaction:

$$10^{-9} - 10^{-3} \left(W / cm^2 \right) \Rightarrow \text{Obtained from normal light sources}$$

High resolution spectroscopy for structure of atoms and molecules

$$10^3 - 10^9 \left(W / cm^2 \right) \Rightarrow \text{Obtained from laser sources}$$

Multi-photon processes, Multi-step excitation processes, Nonlinear optical processes, Rydberg and Autoionizing Levels, Ultra-trace analysis (single atom detection),

$$10^9 - 10^{15} \left(W / cm^2 \right) \Rightarrow \text{High intense laser pulse sources}$$

Intense field regime, Above threshold ionization, Multiple ionization, High harmonic generation (up to 300), Coulomb explosion, Atomic Stabilization

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Spectral Resolution used for spectroscopy:

$$\sim 10^{-3} Hz$$

Ultra precision measurements, Atomic Clocks of accuracy 1 in 10^{16} and better, Ultra-precision magnetometry ($10^{-15} Tesla$ detection)

$$\sim 100 Hz - 10^6 Hz$$

Parity violation experiments in atoms and molecules (non-accelerator particle physics), Study of hyperfine interactions, Hyperfine structure and Isotope shifts, Measurement of properties of unstable nuclei (Nuclear Physics via Atomic physics), Cold atom physics

$$\sim 10^6 - 10^9 Hz$$

Fine structure in atoms and molecules, Atomic & molecular Interactions, State selective processes in atoms and molecules

$$\sim 10^9 - 10^{15} Hz$$

Spectrochemical analysis, Material characterization, Photoionization and photo-fragmentation, supercontinuum sources and their interactions

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Excitation sources used for modern research:

Table-top instruments to high energy particle accelerator

Lasers : 10^{-3} eV to 6 eV photons, used for Rotational, Vibrational and Electronic Spectroscopy

Synchrotron Radiation Sources : 5 eV to 1000 eV photons: used to study Valence to Inner-shell processes

Ion Traps and Atom Trap : Used to study precision measurement in neutral atoms to highly charged ions, U+91 in electron beam ion trap, Study of non-neutral plasma

Particle Accelerators : This is used to study the interactions of charged particles of MeV energies with atoms and molecules

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Systems used for investigations:

A few atoms and ions :

Precision measurements on unstable nuclei produced in an accelerator, Quantum Information Processing using atoms

Small sized clusters :

Metallic and semiconductor clusters, Au_{40} , $\text{Si}_{20}\text{Ge}_{20}$, Approach to bulk properties, Basic for functional materials

Large sized clusters :

$(\text{H}_2\text{O})_n$, $(\text{Xe})_n$, etc, $n = 1000 - 5000$

Used to understand the Van der Waals complexes, solvent interactions in gas phase

10^3 number of cold atoms or ions :

Cold atom physics, Bose Einstein Condensation etc

Gas/liquid phase :

Spectroscopic analysis, trace analysis, pollution detection, chemical and biochemical interactions

In the following, some revolutions in the field of research and applications are highlighted

- The advent of laser opens up a new arena in many disciplines of science and technology.
- The power and precision of lasers have revolutionized the field of atomic physics and molecular physics.

For example, lasers have made possible entirely new technologies for isolating individual atoms in electromagnetic traps and cooling them to near absolute zero. This is known as Laser Atom Cooling.

The Nobel Prize in Physics 1997 was awarded jointly to Steven Chu, Claude Cohen-Tannoudji and William D. Phillips "for development of methods to cool and trap atoms with laser light".

Briefly, when the atoms are brought essentially to rest in the trap by using laser, they can undergo a quantum mechanical phase transition to form a superfluid.

This is known as a Bose-Einstein condensation, while remaining in the form of a dilute gas. This is a new state of matter where all the atoms are in the same coherent quantum state. As a consequence, the atoms lose their individual identities, and their quantum mechanical wavelike properties become dominant.

This coherent beam of atoms can be used to form an "atom laser" analogous to the coherent beam of photons in a conventional laser.

The potential of this future technology hopefully can be exploited for the fabrication of microelectronic and other nanoscale devices.

This can well be used for the development of quantum computer, the dream of many scientists.

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Due to the high precision of lasers, it dramatically increased the precision with which the characteristic wavelengths of atoms can be measured.

Modern standards of time and frequency are based on measurements of transition frequencies in atomic cesium.

An atomic clock is an oscillator whose frequency is locked to the frequency of an atomic transition

The second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine sublevels $F = 4$ and $F = 3$ of the ground electronic state of cesium 133

As shown in Figure – 1.1, the two sublevels correspond to parallel and anti parallel orientations of the spins $S = 1/2$ of the valence electron and $I = 7/2$ of the nucleus of the Cs atom

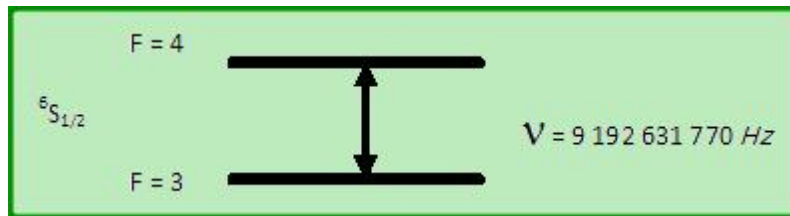


Figure – 1.1

In 1930s, I.I. Rabi and his students, at Columbia University invented this technique known as magnetic resonance, by which they could measure the natural resonant frequencies of atoms. Rabi won the 1944 Nobel Prize for his work.

In 1949, Rabi's student Norman Ramsey suggested that making the atoms pass twice through the oscillating electromagnetic field could result in a much more accurate clock. In 1989 Ramsey was awarded the Nobel Prize for his work.

The discovery and the technology development of this atomic clock lead to the most important application in today's world, a global system of navigation known as Global Positioning System (GPS).

Researchers at the Lincoln Laboratory of the Massachusetts Institute of Technology (MIT) were able to determine the satellite's orbit precisely by observing Doppler shift of its radio signal. Since the satellite's orbit could be precisely determined from the ground, it established that positions on the ground could also be determined by homing in on the signals broadcast by satellites.

On June 26, 1993, U.S. Air Force launched the 24th Navstar satellite into orbit, completing a network of 24 satellites known as the Global Positioning System, or GPS.

This incredible new technology was made possible by using the world's most accurate timepieces: atomic clocks that are precise to within a billionth of a second.

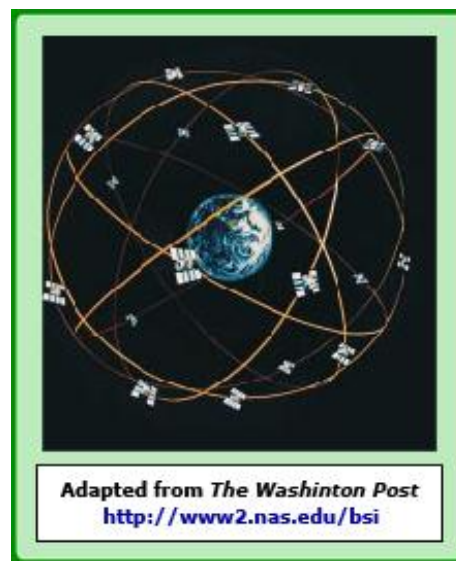


Figure – 1.2

In this system as shown in the Figure – 1.2, there are 24 satellites orbiting 11,000 miles above Earth emits coded signals. Four atomic clocks in each satellite keep accurate time.

Using Doppler shift, receiver on the earth's surface calculates latitude, longitude, altitude, and time by comparing signals from satellites.

This determines the location on the ground, accurate to within 30 meters, or 100 feet.

The Atomic spectroscopy is an important tool in Astrophysics. The analysis of the chemical composition from the spectrum recorded from the heavenly bodies proved many theoretical predictions.

As shown in Figure – 1.3 below, Supernova SN1987A was seen in February 1987. It occurred in Large Magellanic Cloud, 163,000 years ago. Observing the star before the explosion proved the theory that core-collapse of a massive star produces supernova. The spectrum observed from this supernova showed the composition of the star's outer layer. The analysis revealed an over abundance of nitrogen relative to oxygen and carbon as compared to the sun which is the signature of CNO hydrogen fusion cycle.

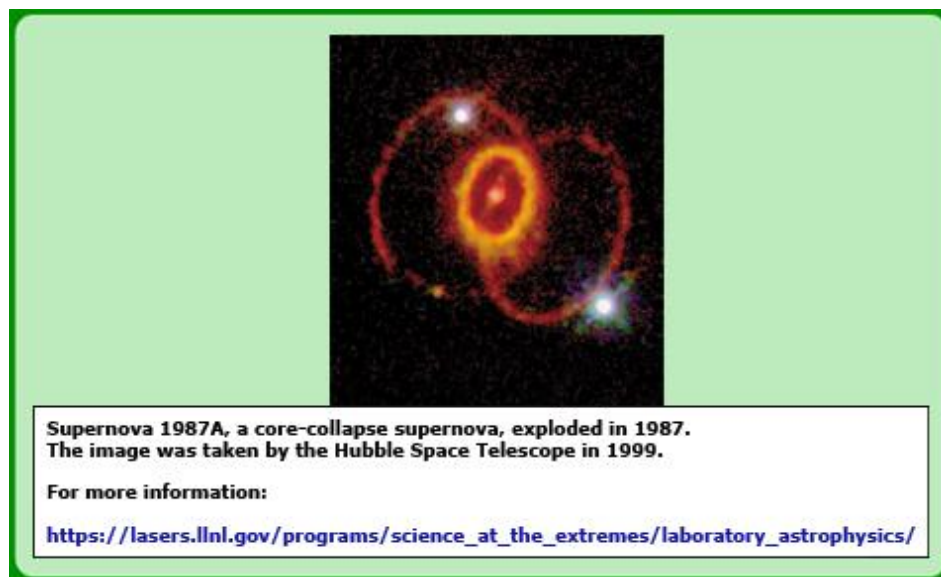


Figure – 1.3

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Plasma, the fourth state of matter is an interesting research field to the scientist. Creating super hot solid plasma state is a challenging task and provides greater understanding of fusion processes.

Researchers working at the U.S. Department of Energy's (DOE) SLAC National Accelerator Laboratory have used the world's most powerful X-ray laser to build the first atomic X-ray laser pulse, as well as to create in a controlled way the superheat (2-million-degree) piece of matter.

The atomic laser could be used to understand the working of biological molecules.

The creation of hot dense matter by intense laser pulse could be exploited to understand the processes of nuclear fusion that power the sun.

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Molecular spectrum is the signature and the fingerprint to identify the molecules. This has a deeper and direct application to our human society.

Now-a-days several spectroscopic methods are used in medical science for diagnosis the disease. In the following, a glimpse of these methodologies is given.

X-rays: the most common instrument used almost everywhere.

The first X-ray device was discovered accidentally by the German scientist Wilhelm Roentgen (1845-1923) in 1895.

He found that invisible rays emitted from cathode-ray tube that penetrate paper and wood but could not penetrate metal and bone. Roentgen used his device to examine the bone structure of the human hand.

X-rays are produced when a target metal (such as tungsten) is bombarded by highly accelerated electrons. These high energy electrons knock out the electrons from the deep energy levels such as K and L shells, the other electrons in higher energy levels occupy these vacant spaces by radiating extra energy in the form of X-rays.

X-rays penetrate the body and the image is stored on silver halide films

Bones and metals absorb or reflect X-rays – leaving the impression on the film, whereas the soft tissues transmit X-rays. This contrast produces an image of bone or metal deep inside the body.

This helps to identify medical problems inside the body such as fractures of bones etc.

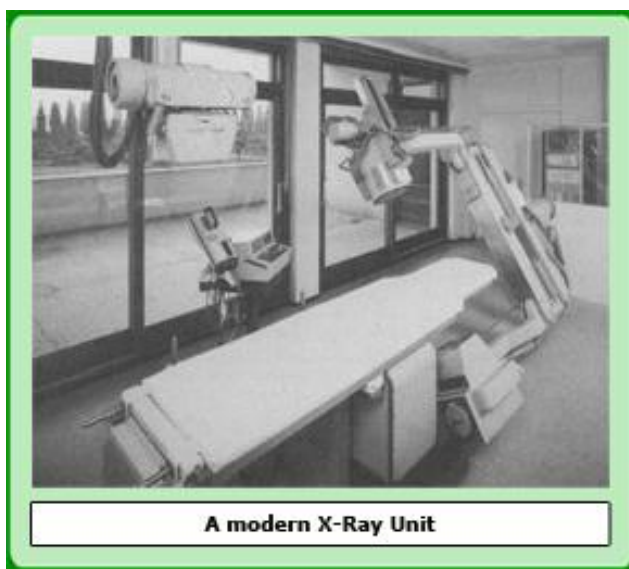


Figure – 1.4

CT Scan or CAT Scan

The scanning mechanism is incorporated by involving a moving target or by revolving the X-ray source. The scintillator, detector for X-ray, is used to pick up the signal and produced the image. By superimposing several images, 2-dimensional and 3-dimensional images are computed.

Positron Emission Tomography

This device measures the metabolic activity by measuring the decay of the radioactive traces injected from outside in tissues. Fluorine 18 is used as radioactive element.

Diseased organs process the injected FluroDeoxyGlucose (FDG) at a higher rate than the normal tissues. Positrons are emitted by FDG and emit g-radiation when collide with electron. g-detectors pick up the signal and compute a 3-dimensional image of the body.

In this way, this methodology helps to identify the location of the diseased organs deep inside the body.

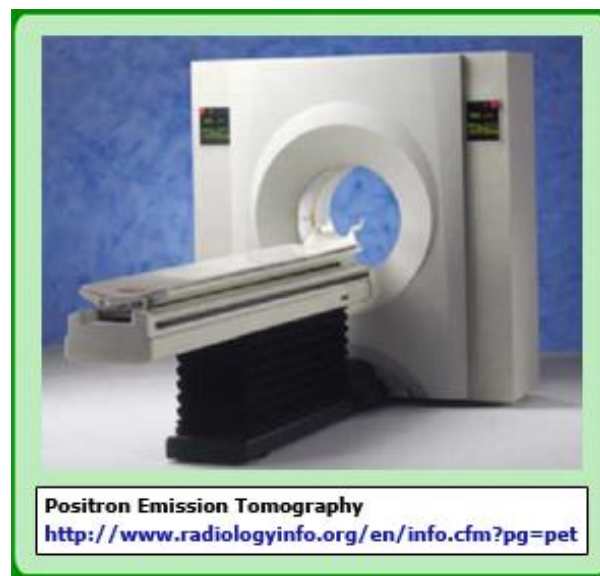


Figure – 1.5

As shown in the Figure – 1.5, the scanner is typically a large, box-like machine with a hole, or short tunnel, in the center. The X-ray tube is rotated and electronic detectors are located opposite each other in a ring, called a gantry. The computer workstation processes the imaging information.

Raman Spectroscopy in medical science:

When the monochromatic light interacts with molecular vibrations, phonons or other excitations in the system, it results in the energy of the photons being shifted up or down. The shift in energy gives information about the vibrational modes in the system.

The Raman Effect occurs when light interacts with a molecule. The light excites the molecule from the ground state to a virtual energy state. When the molecule relaxes it emits a photon and it returns to a different rotational or vibrational state. The difference in energy between the original state and this new state leads to a shift in the emitted photon's frequency away from the excitation wavelength.

Raman spectroscopy is an invaluable technique for investigations of pharmaceutically and medically relevant molecules. It is used in many fields where non-destructive microscopic chemical analysis and imaging is required.

Both Biologists and Chemists use Raman Spectroscopy to identify chemical compounds, their functional groups, and to determine the conformation of complex biomolecules, such as proteins and DNA.

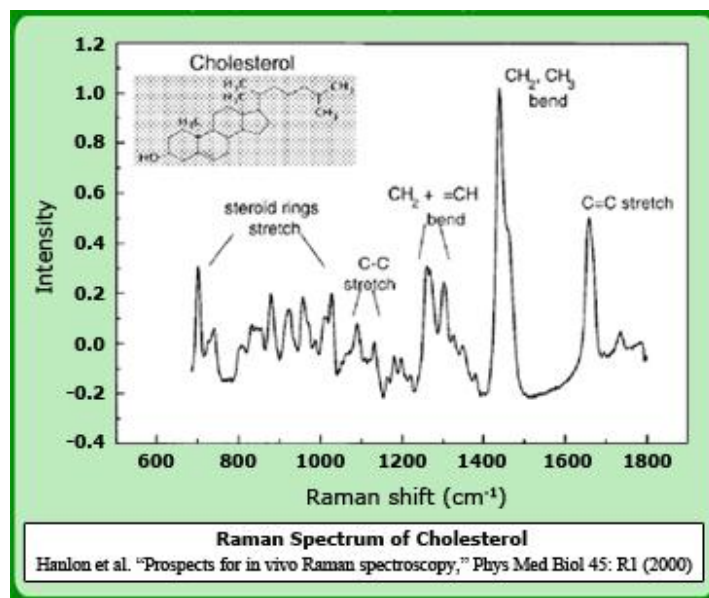


Figure – 1.6

As shown in the the figure – 1.7, the Raman and Surface Enhanced Raman Spectra can be exploited for biosensors.

1. The Raman spectrum of DTNB (1 mM DTNB in d₂H₂O);
2. SERS spectrum of BSA-IgG-AuNP;
3. SERS spectrum of TNB-BSA-IgG- AuNP. Radiation of 633 nm was used for excitation.

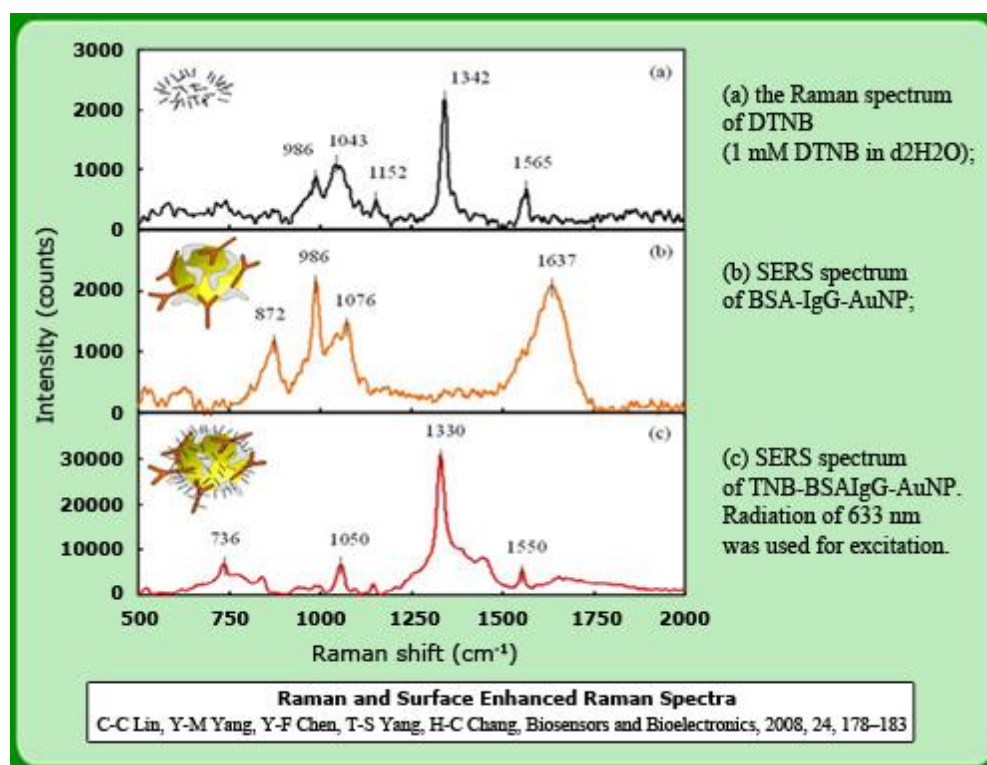


Figure – 1.7

Nuclear Magnetic Resonance (NMR) / Magnetic Resonance Imaging (MRI)

A nucleus with non-zero spin has angular momentum and a magnetic moment such as ^1H , ^{31}P , ^{13}C , ^{19}F

This nuclear magnetic moment interacts with the external magnetic field.

In resonance condition, this absorbs the energy.

To obtain the image: vary the external field as a function of position to localize signals.

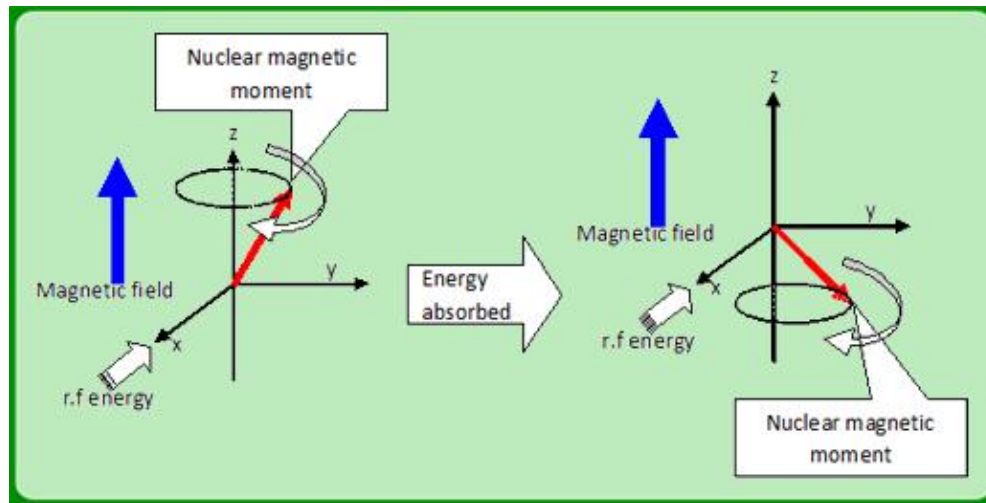


Figure – 1.8

This method is used to acquire the image inside the body especially inside the brain. Having the image from different angles, the medical problems are located.

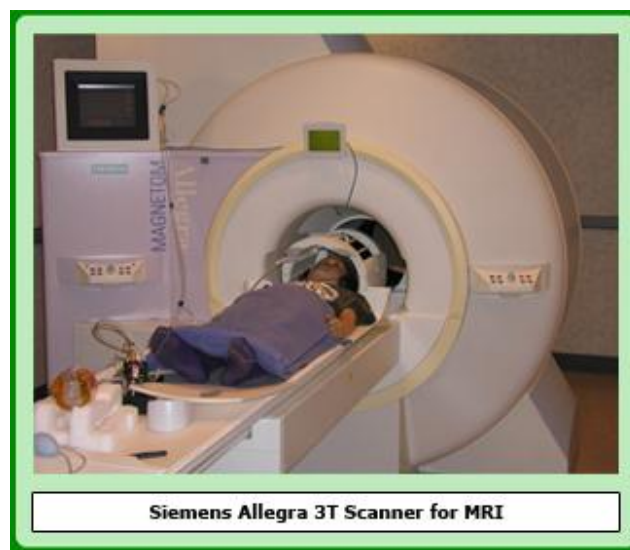


Figure – 1.9

“Matter is made of fundamental building blocks”, idea came from ancient Greeks.

They speculated that earth, air, fire, sky and water might form the basic elements from which the physical world is constructed.

They also developed various schools of thought about the ultimate nature of matter. Perhaps the most remarkable was the atomist school founded by the ancient Greeks Leucippus of Miletus and Democritus of Thrace about 440 bc.

For purely philosophical reasons, and without benefit of experimental evidence, they developed the notion that matter consists of indivisible and indestructible atoms.

Today, we have come a long way developing many thoughts and ideas, carrying out several experimentations and producing lot of evidences.

An understanding of the structure of atoms and molecules is therefore a prerequisite for entering into several of the areas discussed earlier.

The basic atomic and molecular physics is the scientific study of the structure of the atoms and molecules, its energy states, and its interactions with other particles and with electric and magnetic fields.

Recap

In this lecture, we have understood the importance of the Atomic and Molecular Physics.

This subject is important to understand for the development of Quantum Physics.

The basic research in this field of research helped to develop methodology to understand the insight of many other fields of research.

The concept developed in this field helped to develop many devices for medical and household applications.

In the following lectures, we will go through the chronological development of the subject starting from 400 BC.