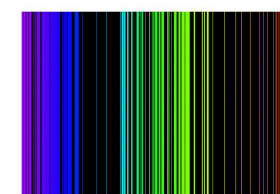
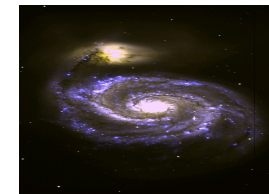
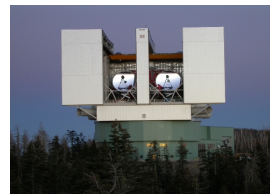




THE OHIO STATE UNIVERSITY



Supercomputer
Center



Research based online course:

**”Atomic and Molecular Astrophysics and Spectroscopy
with Computational workshops on R-matrix and
SUPERSTRUCTURE Codes II”**

**- PROF. SULTANA N. NAHAR,
PROF. ANIL K. PRADHAN**

Astronomy Department, Ohio State University, USA



THE OHIO STATE UNIVERSITY



A.P.J. Abdul Kalam STEM-ER Center
(Indo-US collaboration)

- Organized under the Indo-US STEM Education and Research Center of OSU-AMU, AMU, Aligarh, India, & OSU, Columbus, USA

Oct 4 - 26, 2025

Support: OSU, OSC, OSU-AMU STEM ER Center, AMU



Research training course on "Atomic and Molecular Astrophysics and Spectroscopy with computational workshops on the R-matrix, SUPERSTRUCTURE codes" under the Indo-US APJ Abdul Kalam STEM Education and Research Center of Ohio State University (OSU)-Aligarh Muslim University (AMU), by Prof. Sultana N. Nahar (Email: nahar.1@osu.edu) with guest lecturer Prof. Anil K. Pradhan (AKP, pradhan.1@osu.edu), Dept of Astronomy, OSU, USA

- Lectures & Workshops: 4 weeks, Saturdays & Sundays, 3 hours/session, Oct 4 - Oct 26, 2025
- Venue: online zoom platform. Time: 10 am - 1 pm, US Eastern time
- Computational Facility (online): Ohio Supercomputer Center (OSC), USA

Course certificates (completion/participation w/o exam) will be provided. Participation is free

- Textbook: "Atomic Astrophysics and Spectroscopy" -By A.K. Pradhan and S.N. Nahar (Cambridge University Press, 2011)
- Contacts: Prof. Tauheed Ahmad, Director, Indo-US STEM Education & Research Center, AMU, India Email: ahmadtauheed@rediffmail.com, Mobile: 91-8279632366, 9837404077, SNN: nahar.1@osu.edu

SYLLABUS

Week 1 (Oct 4,5, 2025): Plasma, Atomic Structure, Computational Workshop

- i) Light and Matter, Plasma Sources, Particle and Photon Distributions, Overview on Applications: Chemical abundances, exoplanetary atmospheres, opacities, nano-biomedical X-rays. etc.
- ii) Atomic Structure: Hydrogenic & Non-Hydrogenic Spectra
- iii) Hartree-Fock, Dirac, Breit-Pauli Approximations
- iv) Computational Workshop: SUPERSTRUCTURE

Week 2 (Oct 11,12): Radiative & Collision processes, Computational Workshop

- i) Atomic Process in Plasmas - Radiative Transitions, Electron-Impact Excitation (EIE),
- ii) Photoionization, Electron-Ion Recombination
- iii) Close-Coupling Approximation and R-matrix Method
- iv) Computational Workshop: SUPERSTRUCTURE
- v) Computational Workshop: R-matrix

Week 3 (Oct 18,19 2024): *Computational Workshop on photoionization using R-matrix codes, Molecular Structure & Spectra*

- i) Prof. Pradhan lecture: Molecular Structure and Astrophysical Spectra
- ii) Photoionization, radiative transitions using R-matrix method
- iii) Computational Workshop: R-matrix calculations for photoionization

Week 4 (Oct 25,26, 2025): *Astrophysical Applications, Exam, Certificate*

- i) Prof. Anil Pradhan's lectures: Plasma modelling and Plasma opacity
- ii) Review of materials
- iii) Exam and evaluation
- iv) Preparation and distribution of Certificates by Nov 7, 2025

NOTE: Computational workshops on R-matrix method are divided in two parts

- Part I: Collisional excitation and Part II: radiative processes

- Present form: Part II: Computation will focus on Photoionization and Oscillator Strengths

GLOBAL PARTICIPATION REGISTRATION:

- To enroll, email the following information (the way you want for the certificate)

Full official name:

Designation (Prof, Dr., Researcher, Student with current status of education):

Name of the affiliated University or Institution:

City and country names:

Email:

- zoom link for the sessions:

<https://osu.zoom.us/j/9111111111>

Personal meeting id: 665 664 7991, pw: 330775

- Please create your account at Ohio Supercomputer Center (OSC) following the instructions in the next pages. Note: OSC will provide a new access code.
- OSC may have changed some options during the past year. Any issue can be solved by contacting OSC at oschelp@osc.edu

Get your account at Ohio Supercomputer Center (OSC)

For the computational workshops, you will need an account at OSC. Please follow the steps below from the weblink

- https://www.osc.edu/supercomputing/portals/client_portal/self_signup_for_accounts

- Click on blue highlighted link "MyOSC" right below "Self-Signup for Accounts"

It will open up to a window for "log in" and "Sign-up". For new account click on "Sign-up" which will open up "Your Contact Information" page

Enter your information (Red asterisk boxes).

If you do not have institutional email address, put down the email address that you have. Click on the "Submission" bar.

OSC will send you an email with a code to verify your email address. It will also open a window to type that code from your email. So check your email to get the code and put it in the box "Enter your Code here". - Click in the box "I'm not a robot". You get a CAPTCHA image to click on boxes

This will go to the next page with you will enter your access code:

- Project code: PAS1866

- Access code: 312890 (Expires: 14-OCT-25)

- To login to your account, you will go to the same page of "myosc portal".

Please remember to use Project code and the Access

- To log in to you account from a "terminal window". Follow as:

- Type: `ssh YourID@owens.osc.edu` (ssh app could already be in your computer)

- or: `ssh -o serveraliveinterval=60 YourID@pitzer.osc.edu`

The option "-o serveraliveinterval=60" lets you stay logged in for a longer time.

Please note that after typing each command, you will hit the <return> key

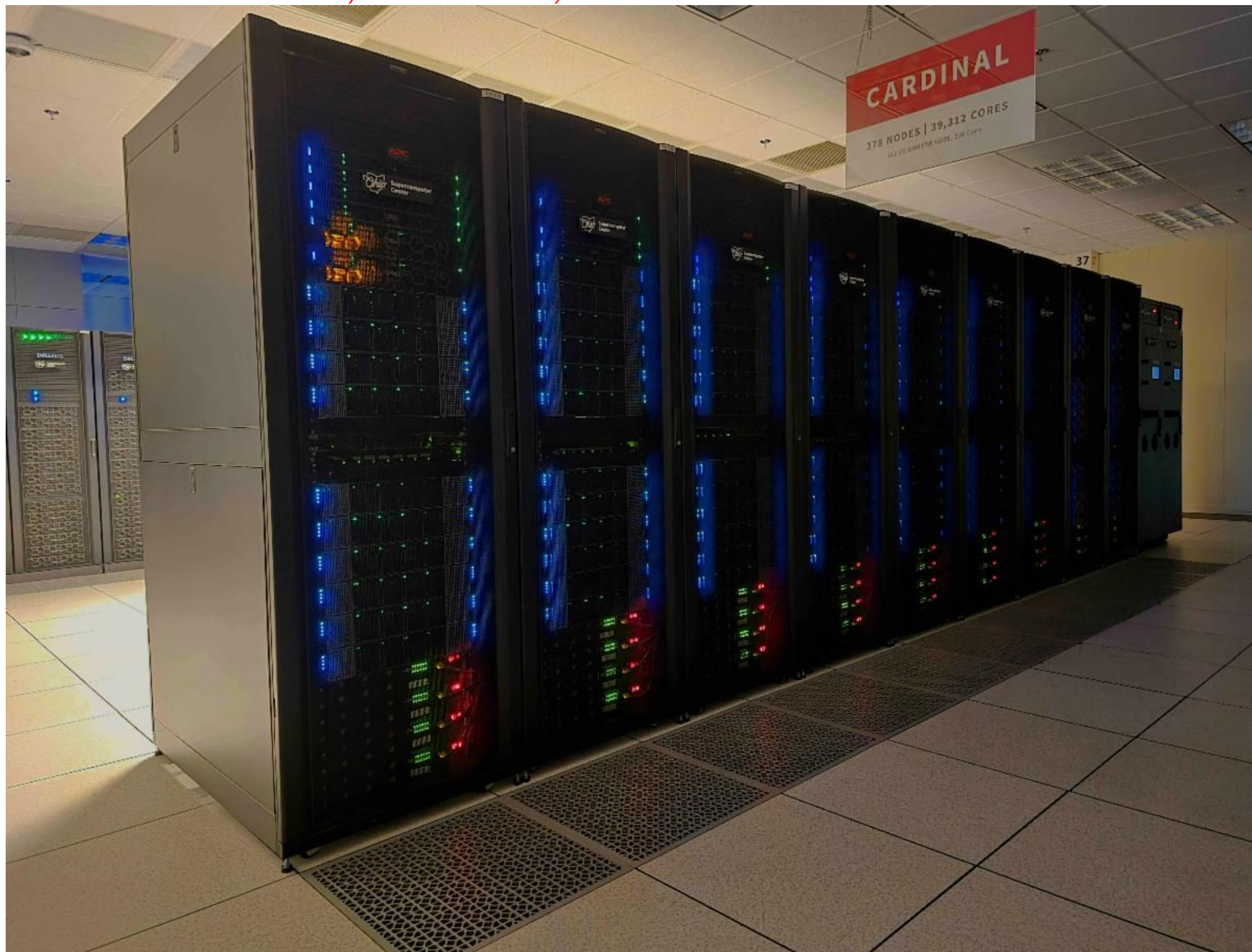
Log in to you OSC account for running jobs

For the computational workshops, you will need a terminal window where you can write commands for viewing and editing files, submitting and running programs.

You can use any of the following terminals:

- i) The terminal window that exists in your computer
- ii) Download from the internet "Putty" which creates a terminal window to log in to a remote host
- iii) use the terminal window that OSC provides from "onDemand" log in page. For the OSC terminal, please follow the steps below:
 - On the internet, go to: <https://ondemand.osc.edu>
 - Click on "OSC OnDemand - Ohio Supercomputer Center"
 - OSC log in page will open up.
 - Type in your user name and password and click on the bar stating "Log in with your OSC account"
 - You will be led to your account page
 - From the top blue bar, click on the "Clusters" and drag your cursor to "Pitzer shell access".
 - This will take you to the terminal window to work (black background)
 - Work on your programs: copying, running, check the input output files etc.
 - When done with your work, go to the previous page by clicking on the "Dashboard OSC" box at the top bar of your browser
 - On the right of the top bar on you account page, you will find "log out" to click and get out.
 - For any issue, contact OSC at: oschelp@osc.edu

- HPC cluster, Cardinal, at OSC



- Download the book from free websites

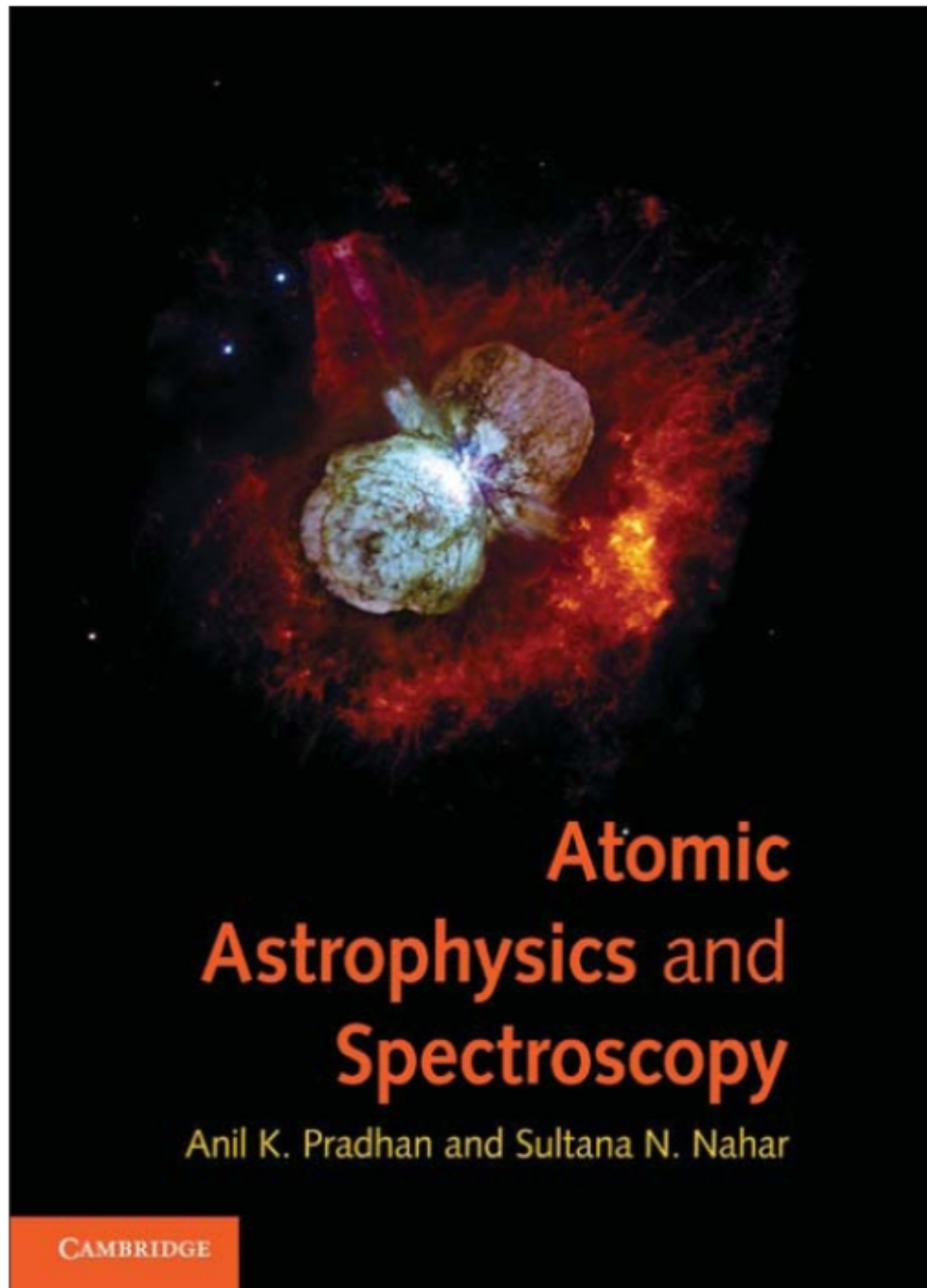


Table of Contents

1. Introduction
 2. Atomic structure
 3. Atomic processes
 4. Radiative transitions
 5. Electron-ion collisions
 6. Photoionization
 7. Electron-ion recombination
 8. Multi-wavelength emission spectra
 9. Absorption lines and radiative transfer
 10. Stellar properties and spectra
 11. Stellar opacity and radiative forces
 12. Gaseous nebulae and HII regions
 13. Active galactic nuclei and quasars
 14. Cosmology
- Appendices



Invite to APS membership:

AMERICAN PHYSICAL SOCIETY (APS)

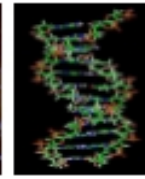
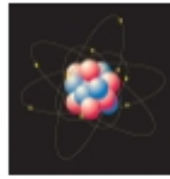
- It is the largest scientific network for physics and related subjects.
- APS journals are Phys. Rev. A, B, C, D, E, PhysRevLett, etc.
- It holds annually two general (Global Summit), and a number of conferences
- It gives many prestigious prizes and awards, and a number of grants
- APS Membership can be free for 4 years and be renewed for developing countries, free for 1 year for any US/non-US student:

Go to Website and click on box "APS/FIP":
<https://www.aps.org/membership/join/physicists-worldwide> or to my page <http://www.astronomy.ohio-state.edu/nahar.1/fip.html>

- Click on "APS MEMBERSHIP link" (<https://www.aps.org/membership-worldwide>) which will take you to APS membership page
- Click on "Apply for matching membership today" under "Apply for matching membership"
- You will taken to page where you will create an account
- Login. You will see the online membership application form. Fill it out. You should hear from APS in a week.
- After becoming member (will receive ID from APS),
 - become a member of your division & of APS unit
 - FIP: Forum of International Physics

Post your resume Sign up for job alerts and apply online

بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ



INTERNATIONAL SOCIETY OF MUSLIM WOMEN IN SCIENCE (ISMWS)

ISMWS CHARTER

Founder: Dr. Sultana N. Nahar

The Ohio State University, Columbus, Ohio, USA

April 19, 2010

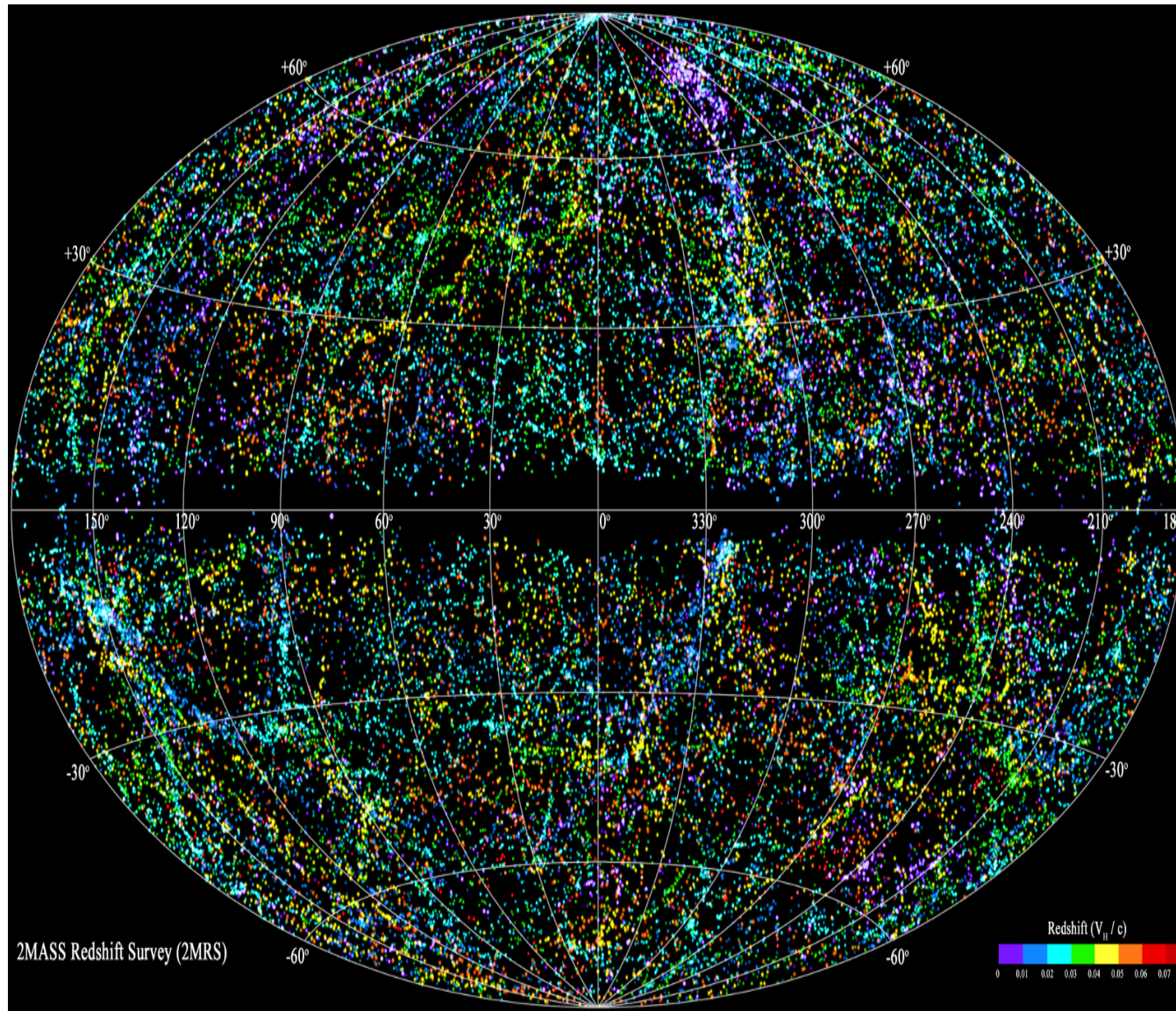
- **AIM:** - encourage Muslim women in science profession, form a network for various support
- **Objective:** Stay in Science (basic or applied)
- **Motto:** Out of 24 hours a day, we keep some hours for our intellectual nourishment
- **Members:** Over 450 from 33 countries & has chapters

Web: <http://www.astronomy.ohio-state.edu/~nahar/ismws.html>

For membership (free) - Email: nahar.1@osu.edu

UNIVERSE through RADIATION:

Most Complete 3D Map of the universe (Created: By 2MASS - 2-Micron All Sky Survey over a decade)



- Includes 43,000 galaxies extended over 380 million light years
 - Redshifts, or measurements of galaxy distances, were added
 - Missing black band in the middle because of invisibility behind our Milky Way
- There are 2 trillion galaxies in the universe

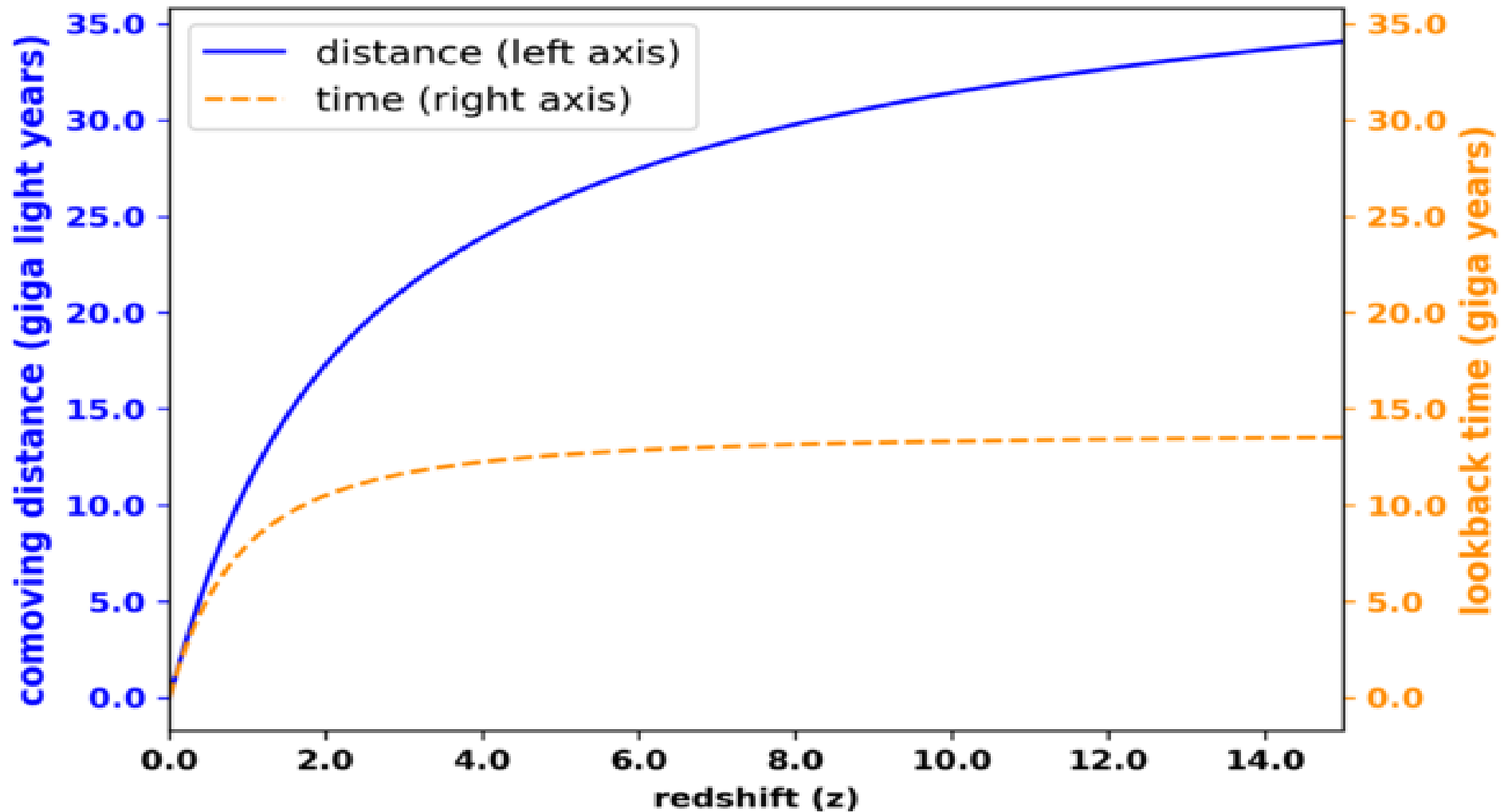
Near empty space: Spiral galaxy NGC 3521 Ours: Milky Way

Distance: Sun & nearest star Alpha Centuri, 4 lyrs



- There are about 2 trillion galaxies in the observable universe. Before Hubble's finding, the Milky Way was assumed to be the whole universe. It is important to study the space & we have a long way to go
- Observable universe size: about 93 billion light years. How do we study the universe? - Through atomic & molecular spectroscopy

Z-REDSHIFT FOR UNIVERSE SIZE: Lookback time



$$z = \frac{\text{Wavelength Observed}}{\text{original wavelength}} - 1$$

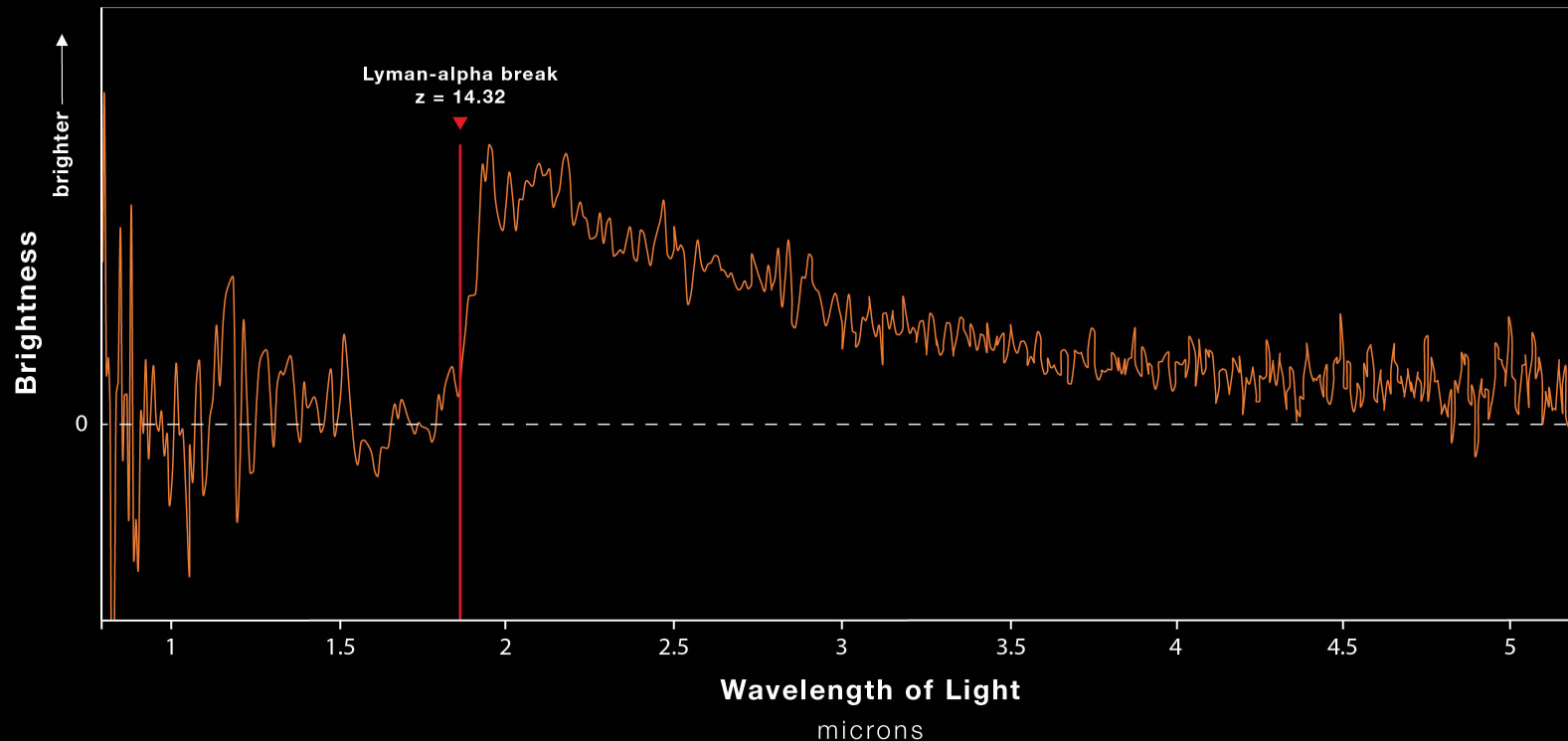
- From an astronomical object spectrum, determine z redshift from Lyman alpha line, 1216 Å, of Hydrogen.
- Use z in Hubble law to get the velocity, $v = c \times z$, and the distance $d = v / H_0$. H_0 = Hubble's constant = 70 km/s assuming universe is expanding at a constant speed. However, considering the universe is accelerating, H_0 becomes variable

HIGHEST Z-REDSHIFT OF A GALAXY: JADES-GS-z14-0 WITH $z = 14.32$

GALAXY JADES-GS-Z14-0

GALAXY EXISTED 300 MILLION YEARS AFTER BIG BANG

NIRSpec Microshutter Array Spectroscopy



with $z=14.2$, lyman alpha line, 1216 Å, stretches to $\lambda_{obs} = \lambda_{rest} \times (z+1) = 18629 \text{ Å} = 1.86 \text{ micron}$.

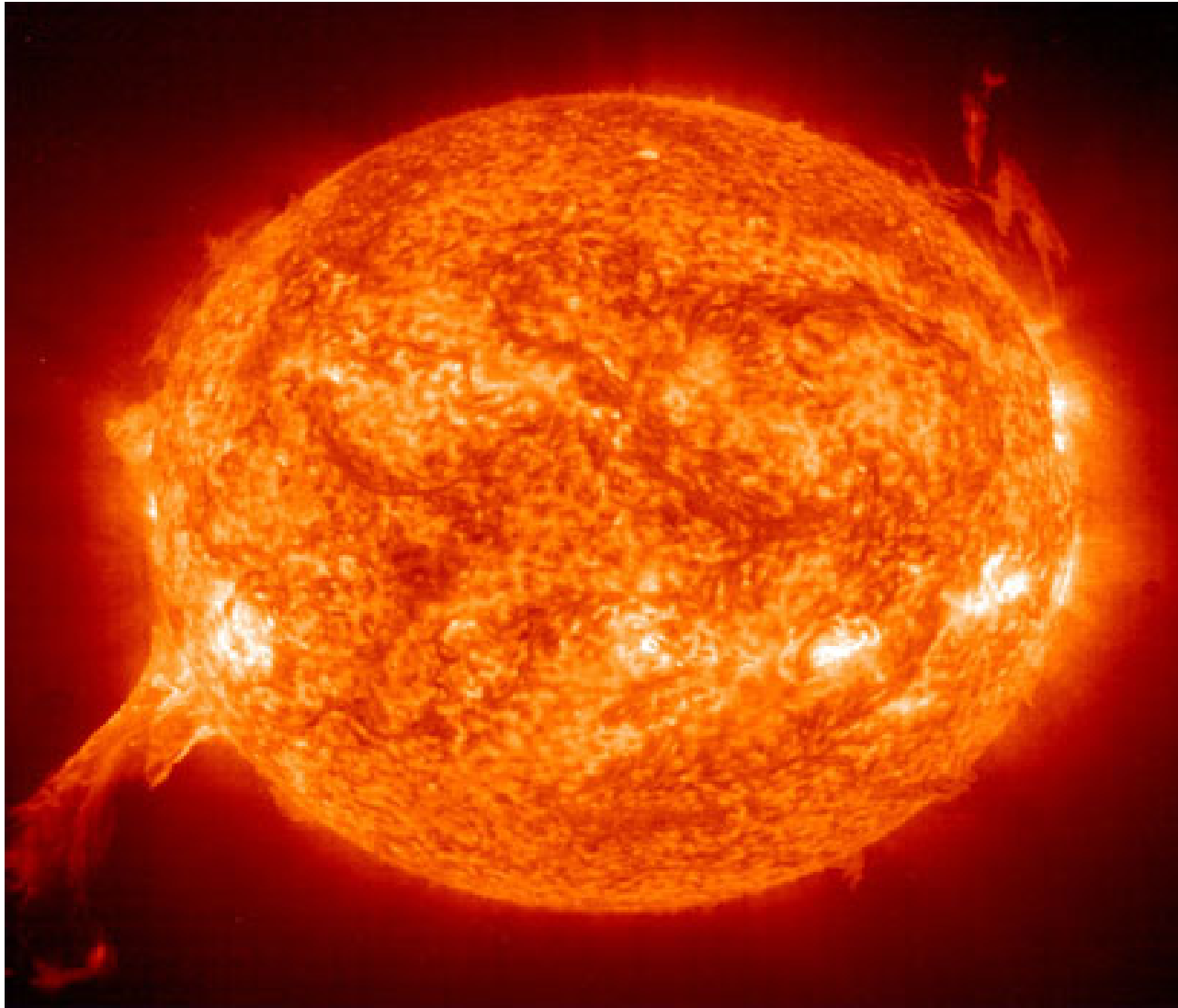
- The largest-observed redshift, corresponding to the greatest distance and furthest back in time, is that of the cosmic microwave background radiation;
- With redshift about $z = 1089$, it shows that universe is 13.8 Byr.

ASTRONOMY: Anything beyond our earth - but important to study. Our galaxy: MILKY WAY (stable)



- Has 200-400 billion stars. About 98% of the stars will lead a life evolution similar to the Sun.
- Milky way is spherical. Crossing over will take (diameter) over 100,000 LY. The Sun is near the edge of it
- Light or radiation is emitted by excited or “HOT” atoms, molecules in them
- Being near edge it avoids risk of being swallowed by a BH.

OUR SUN - The "unQuiet" Star (Observed by SOHO)



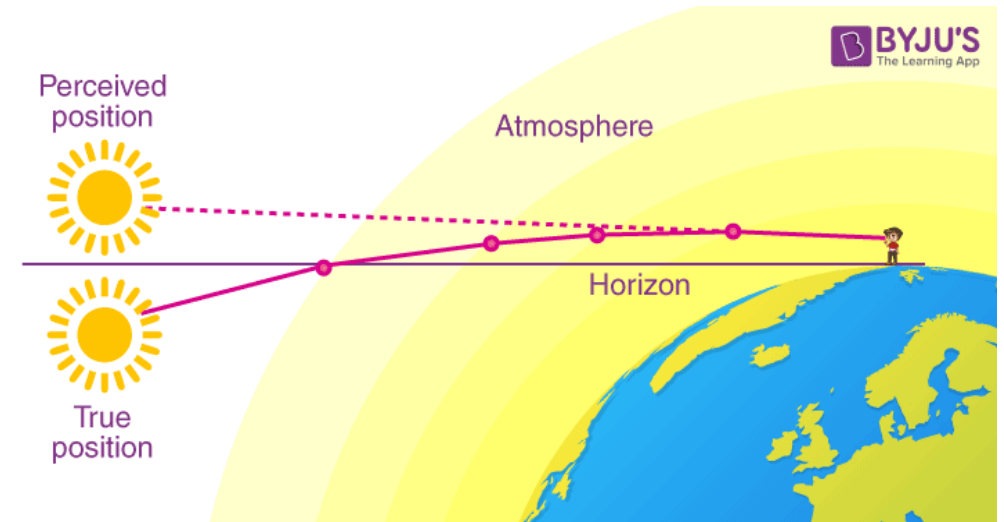
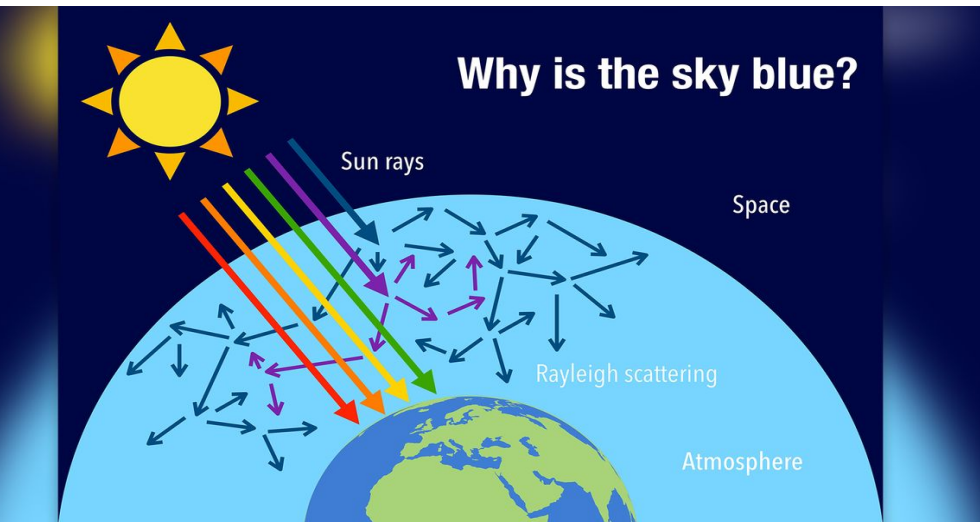
- The Sun - a very dense and hot ball of plasmas
- Sun has a 11 years cycle of minimum to maximum ACTIVITY, when its magnetic field flips between North & South. Pic: White active magnetic regions & flares on the surface. A typical solar flare $\sim$ larger than the earth
- Activity: Eruptions with explosions & ejecting large amount of particles & radiation in to space which can affect the earth

The SUN, our STAR (diameter: 110 x Diameter-earth)



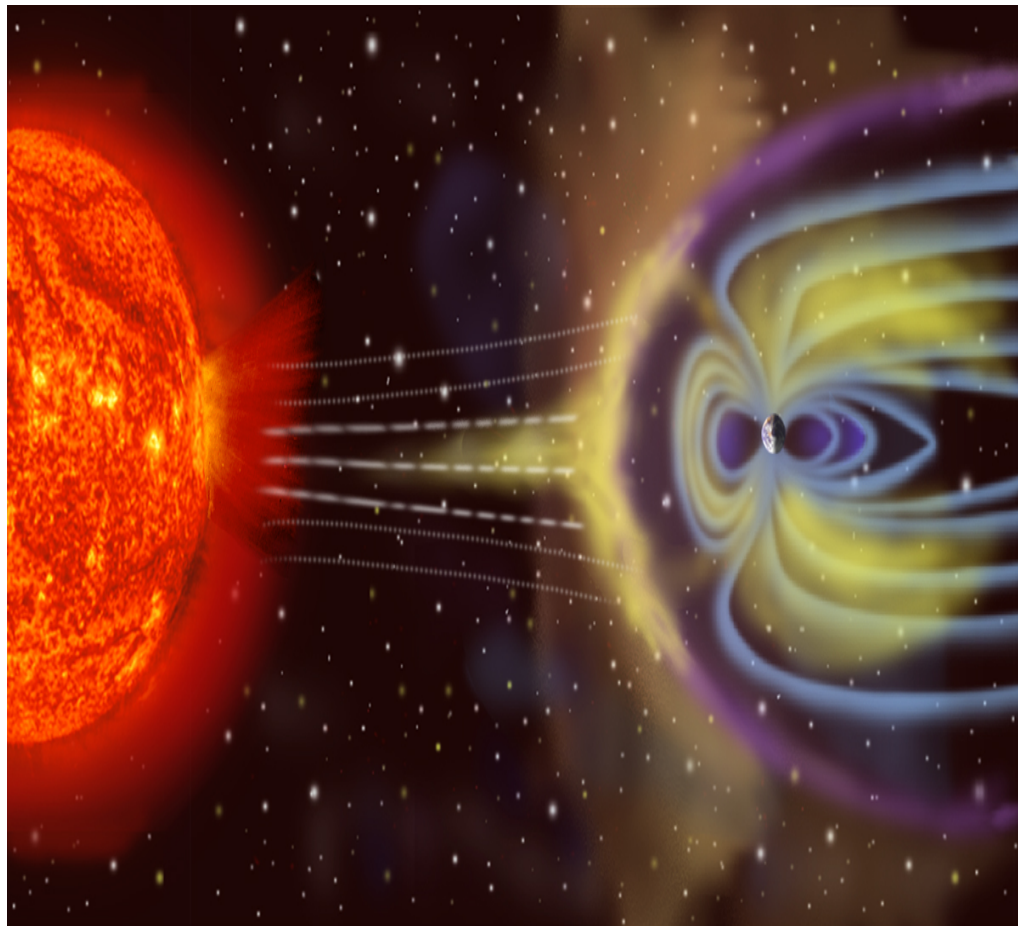
- The Sun has 8 planets (M-V-E-M terrestrial, J-S-U-N gaseous)
- It is an extremely dense and hot ball of plasma, gives out huge amount of radiation, Only small fraction of sun's radiation reaches the earth. The Sun is the source of energy for us

The SUN creates Blue and Red sky, make the Earth beautiful



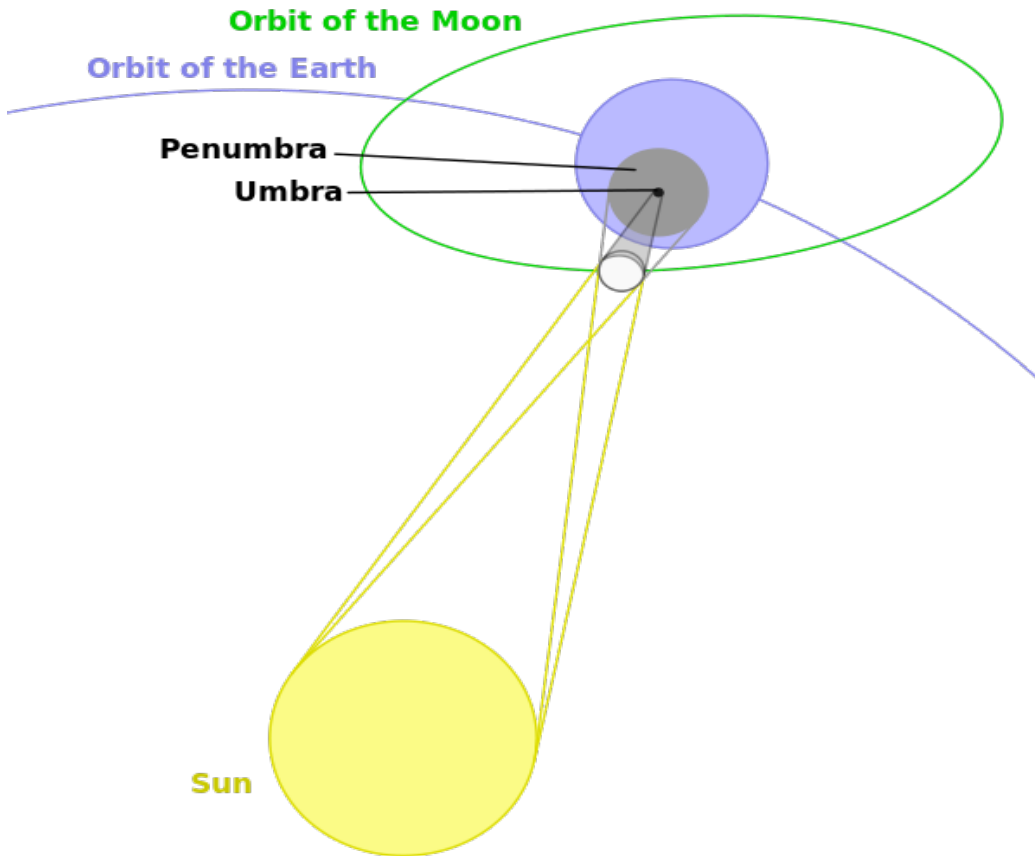
- Sky is blue at high Sun because atmospheric molecules scatter the blue photons to the earth. Blue sky is reflected on the water.
- Sunrise or sunset brings red photons as they bend toward the earth due to refraction travel through layers of atmosphere. This also causes Sun to be seen when it may be below the horizon

The SUN has Solar Storms: Ejects Radiation & Particles



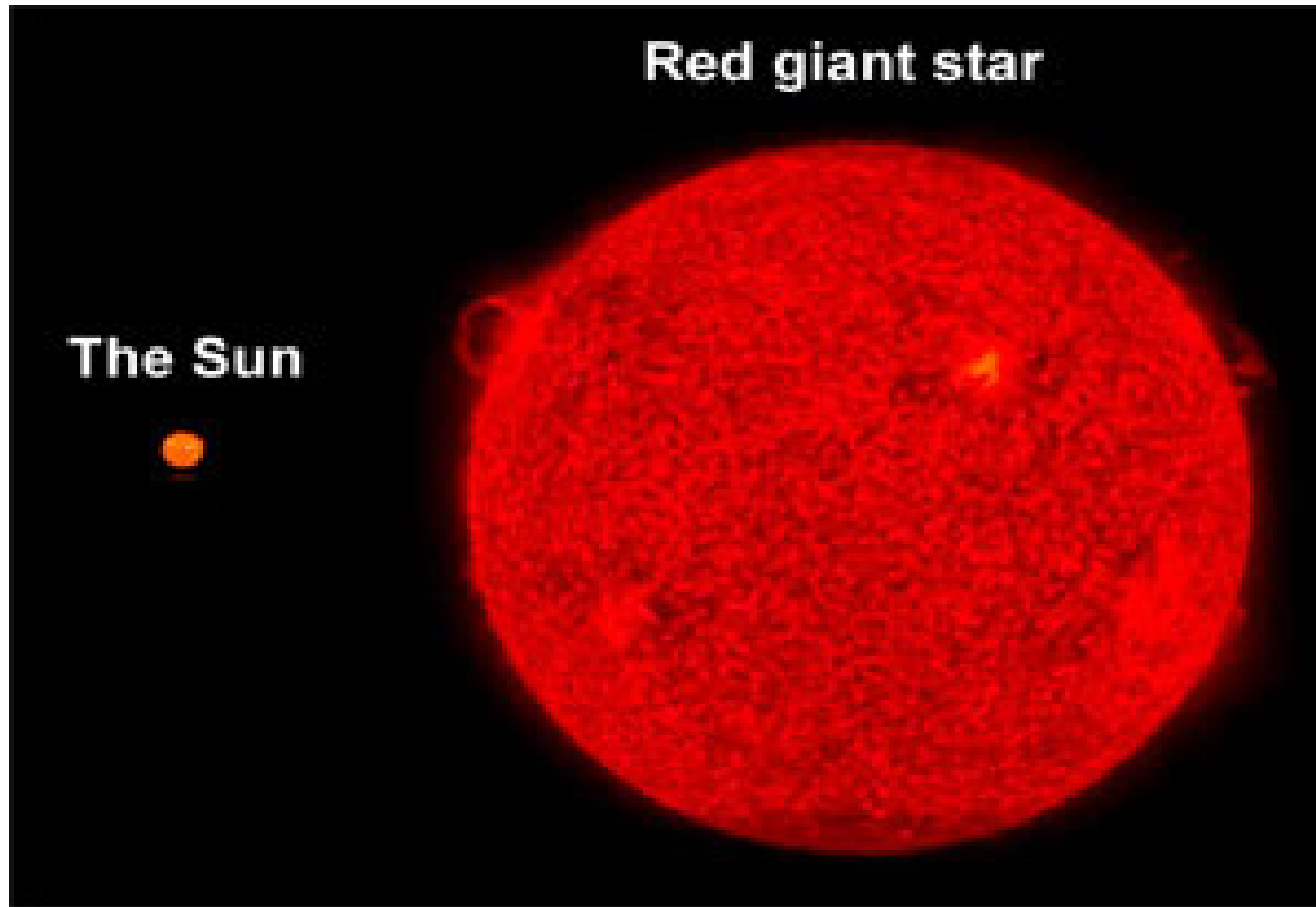
- The active sun with solar spots blasts huge amount of radiation Gamma ray, x-ray, UV, and charged particles in space which are harmful to us. But we are protected:
- i) the atmosphere deflects, burns the particles, ii) ozone blocks high energy radiation, iii) its magnetic field captures the charged particles seen as aurora or the northern lights.

SOLAR ECLIPSE (April 8, 2024)



- Total solar eclipse, a cosmological event of interest, occurs at occasional alignments of the Sun, Earth and Moon.
- Total eclipse gives the scope to see the surrounding of the Sun blocked by Sunlight
- The Sun is surrounded by three outer thin plasma regions: Photosphere (surface to 250 mi, 6500 - 400 K), Chromosphere (250-1300 mi, 4000 - 8000 K), Transition Region (60 mi, 8000 - 500,000 K) and the Corona (1300 - , 500,000 - a few Million K)

LIFE OF OUR SUN: RED GIANT IN 6-7 BYR



- SUN: 4.5 BYr old, live for another 6-7 BYr. The current age of the universe ~ 13.8 BYr
- It will become a Red Giant, a dying expanded star with H fuel gone
- The heat, radiation, electrons will push materials out to form a red giant. • Red giant will slowly become planetary nebulae and ultimately white dwarf. Over 90% stars will end up to white dwarf and lot of diamond in them $\rightarrow$ earth will be engulfed, we will need another home

PLANETARY NEBULAE - Endpoint of a Star [PNe K 4-55]



- Condensed central star: very high $T \sim 100,000 \text{ K}$ ($\gg T \leq 40,000 \text{ K}$ - typical star). Envelope: thin gas radiatively ejected & illuminated by central star radiation: red (N), blue (O). Lines of low ionization states - low ρ & low T
- Ionized gaseous nebulae: associated with birth & endpoint of stellar evolution $\rightarrow$ chemical enrichment is a chronometer of life of the universe itself

End of life: WHITE DWARF - Ex: Diamond white dwarf 2014



- "Astronomers discover Earth-sized diamond-encrusted white dwarf" 2014. It is so old that it has crystallized into a Earth-sized diamond
- A white dwarf is very dense: its mass is comparable to that of the Sun, while its volume is comparable to that of Earth.
- About 98% stars will end up as white dwarfs
- Ultimately they will be black dwarfs after losing all energies

THE 1ST OBSERVATORY, SAMARKAND, 1420, BY MUSLIM RULER ULUGH BEG (Iran has an older model)

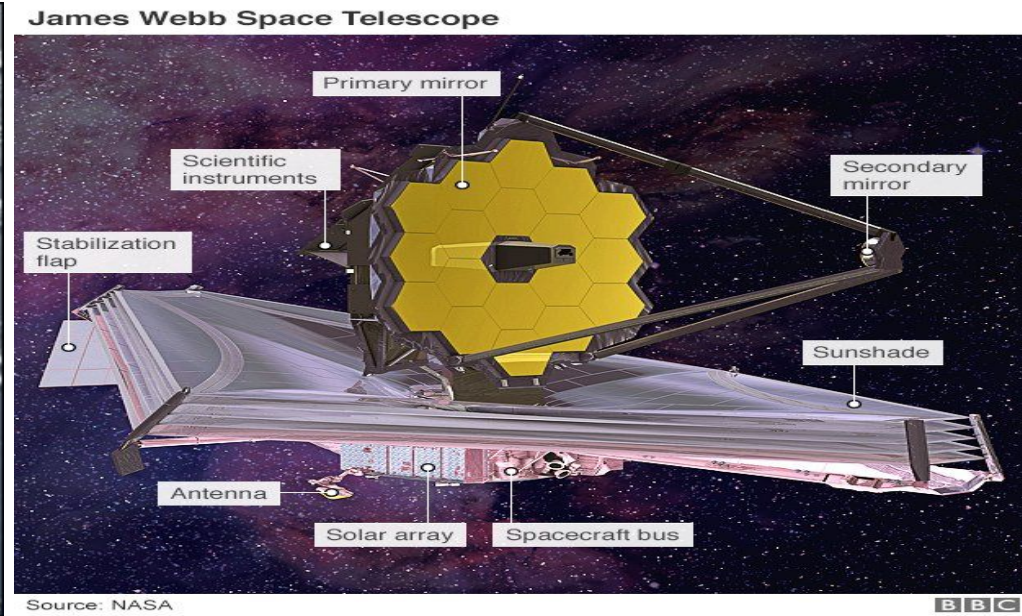


- Ulugh Beg built the madrasa in 1420 in Samarkand and extended it to an observatory
 - Beg himself recorded many astronomical objects.

MODERN DAY GROUND & SPACE BASED TELESCOPES



L: Large Binocular Telescope in Arizona (8.4m Mirrors, NIR-optical), R: Hubble space telescope

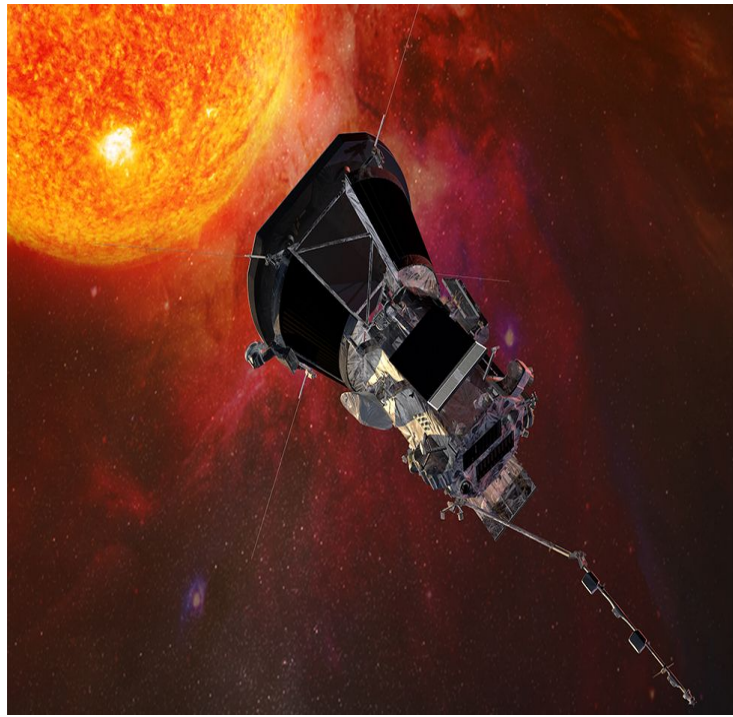


L: International Space station of NASA, R: JWST

How India's Chandrayaan-2 will reach the Moon

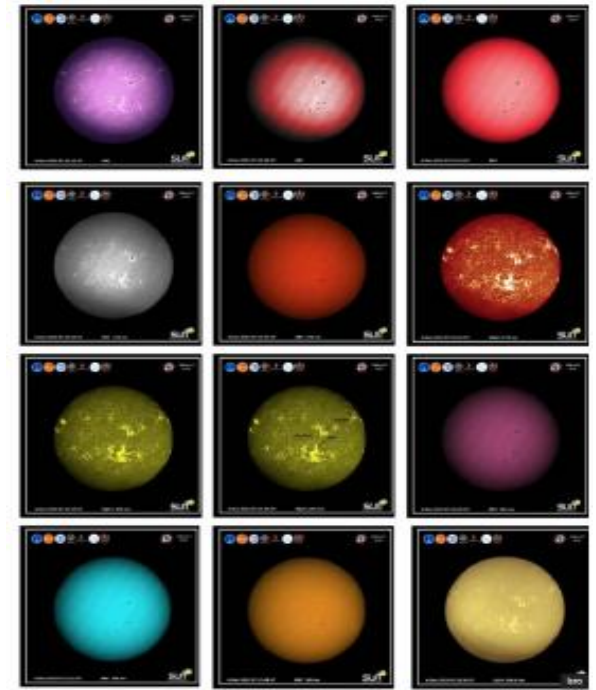
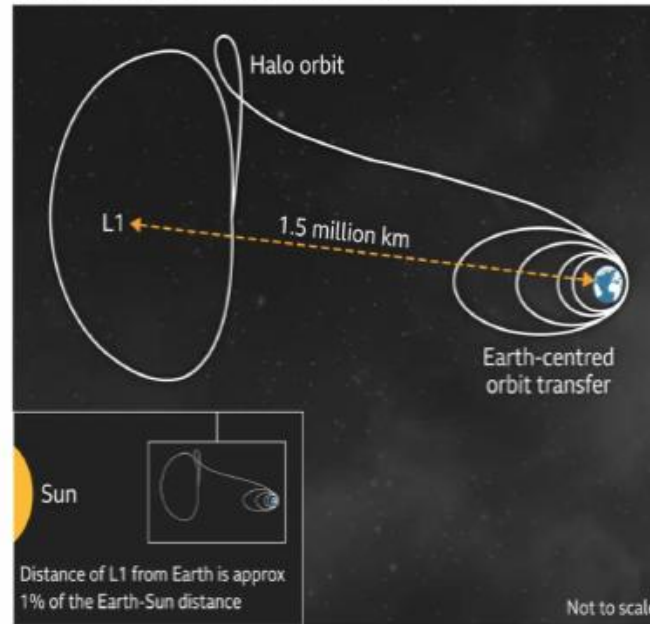
DEDICATED OBSERVATORIES FOR THE SUN

PARKER SOLAR PROBE & ADITYA L1



Aditya-L1 mission trajectory

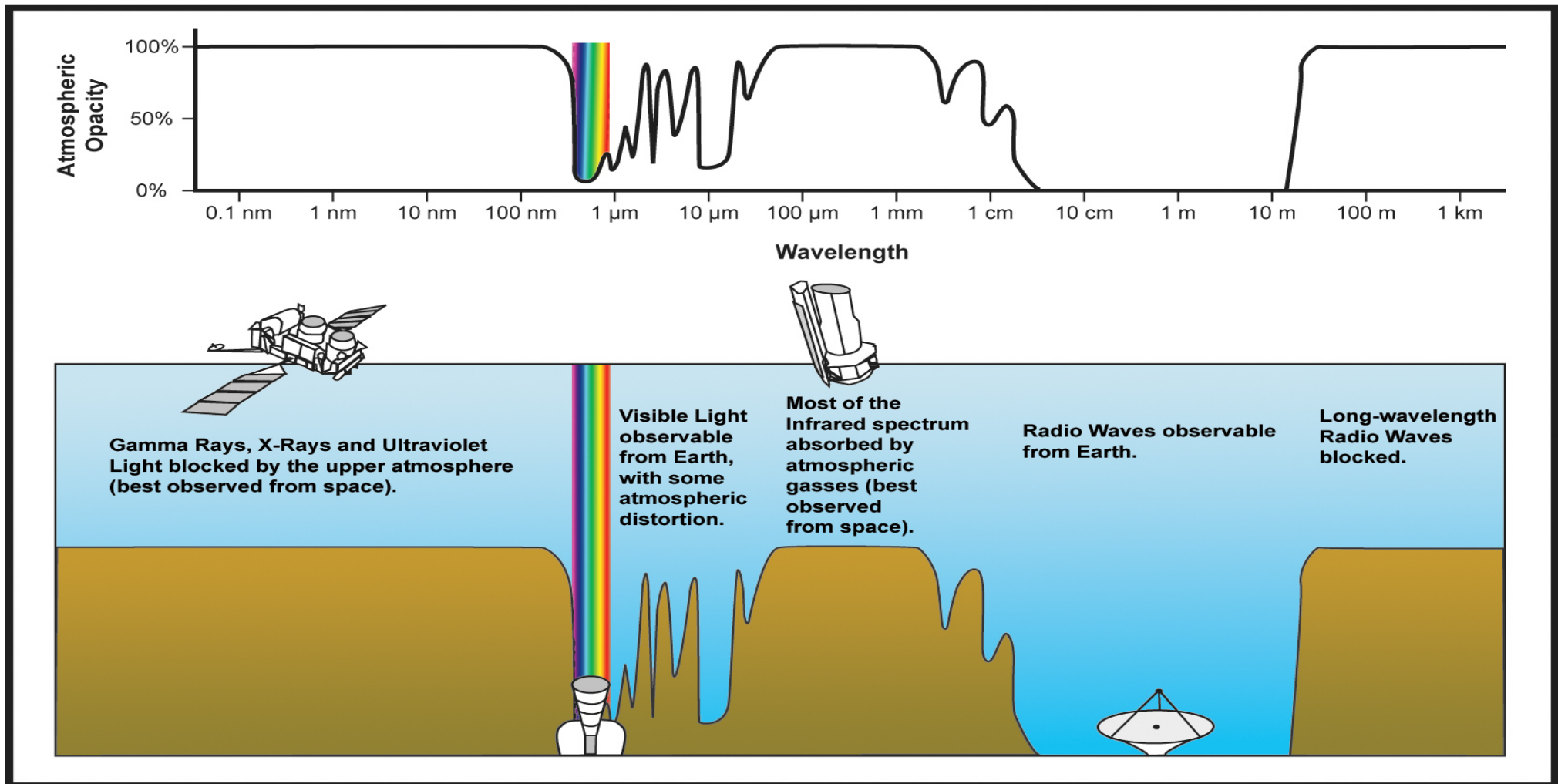
The first Indian solar mission to study the Sun



These images of the Sun sent by Aditya-L1 provide insights into the Sun's photosphere and chromosphere.

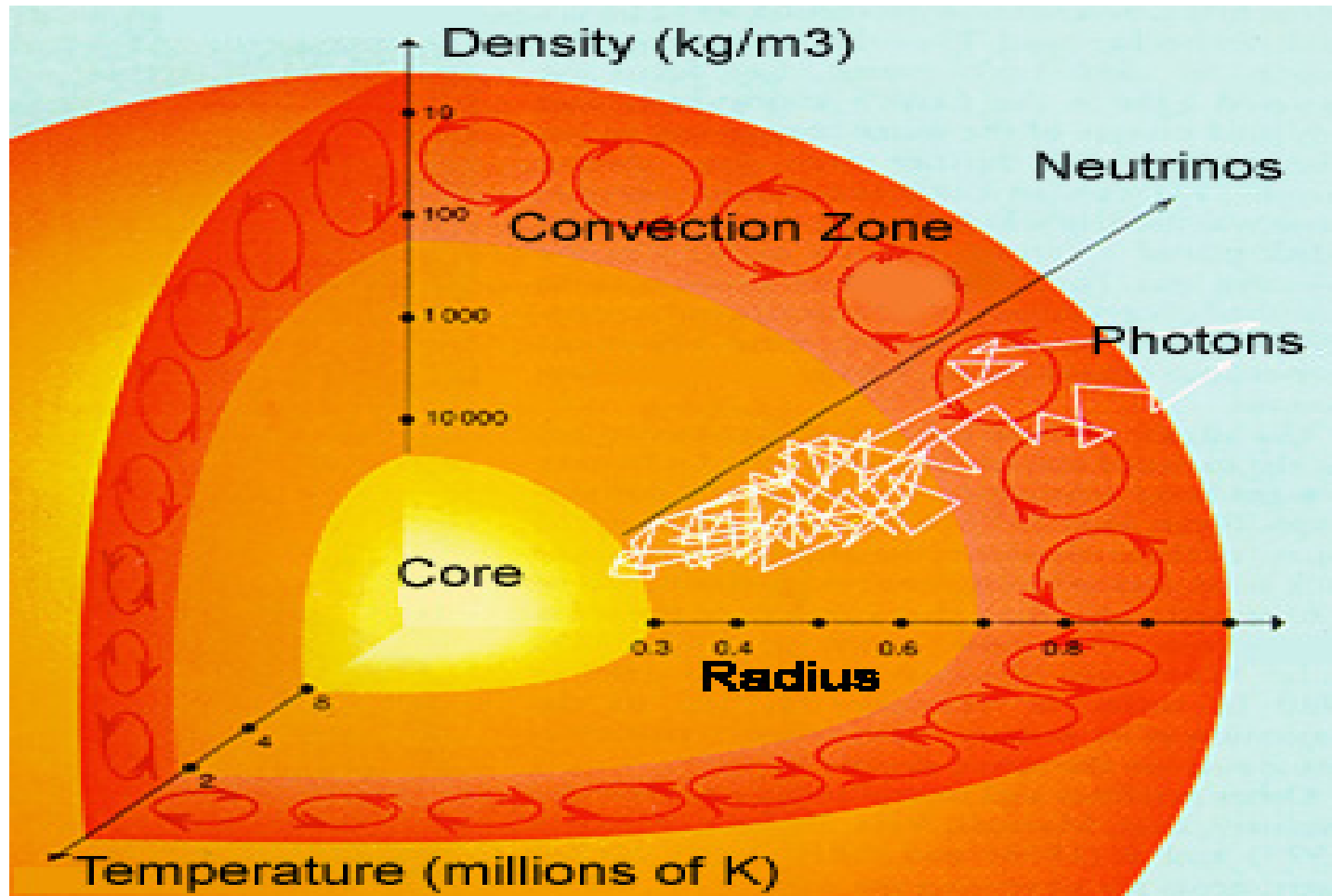
- L: Parker Solar Probe makes historic pass through Sun's atmosphere withstanding intense heat.
 - A satellite/ spacecraft goes around the earth several times, each time making a longer elliptical loop by the gravitational push, until going straight toward the object - path of Indian spacecraft Aditya L1 (Lagrange point 1) to study the Sun.
 - It sent various images of the Sun in corona and chromosphere.

ATMOSPHERIC OPACITY: ABSORPTION OF RADIATION



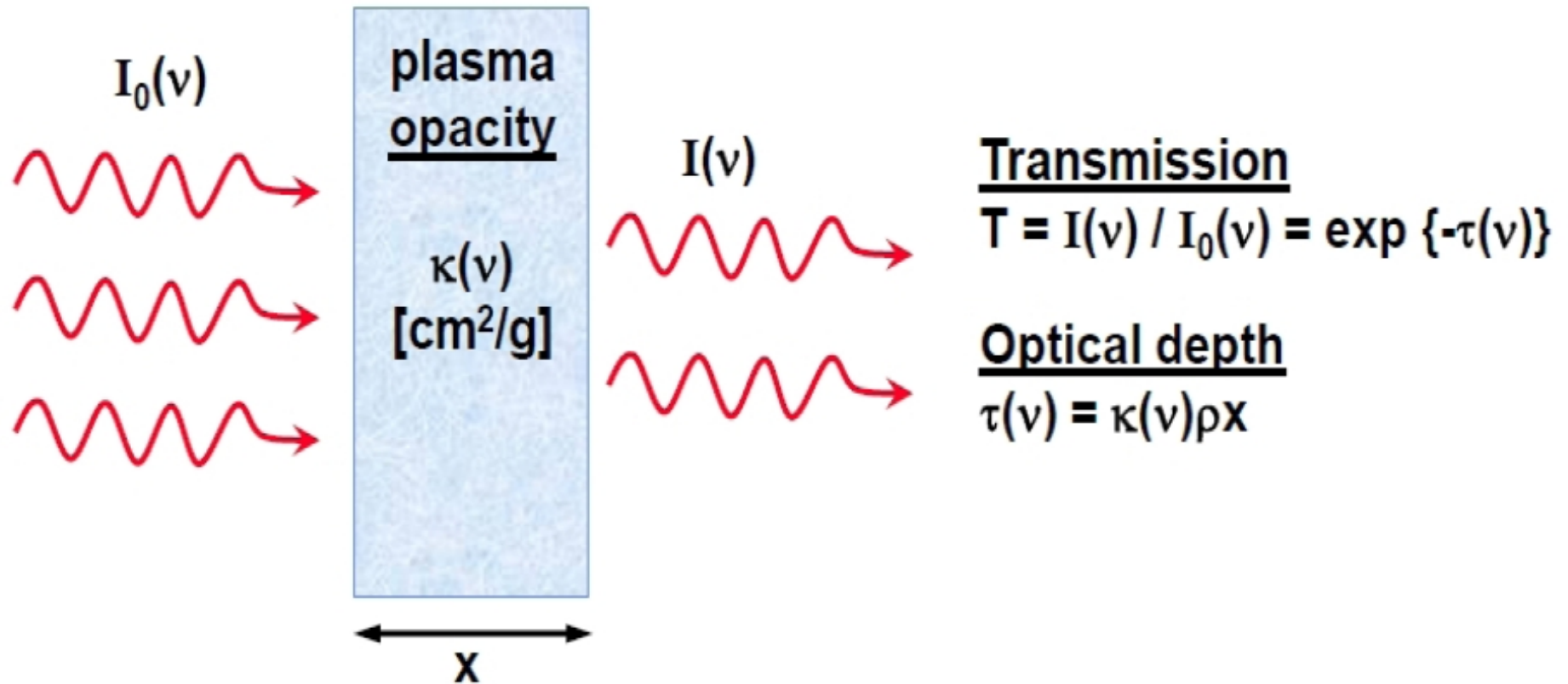
- Higher opacity -less radiation reaching earth's surface
- Opacity determines types of telescopes - earth based or space based
- Gamma, X-ray, UV are blocked while visible light passes through
- CO₂, H₂O vapor, other gases absorb most of the infrared frequencies
- Part of radio frequencies is absorbed by H₂O and O₂, and part passes through

SOLAR PLASMA OPACITY & ELEMENTAL ABUNDANCES



- **3 regions of the Sun:** 1) Core: 15 mK, 150 g/cm³ - nuclear fusion center - H fuses to He & produces gamma rays, 2) Radiative zone - highly dense and hot plasma - energy transfer through diffusion, 3) Convection zone - boiling plasma. **The change in phase between radiative and convection zones is distinct. The boundary distance R_{RC} is known.**
- Absorption of radiation by the constituent elements cause solar plasma opacity and slow down the escape of the radiation. R_{RC} can be predicted from opacity

PLASMA OPACITY

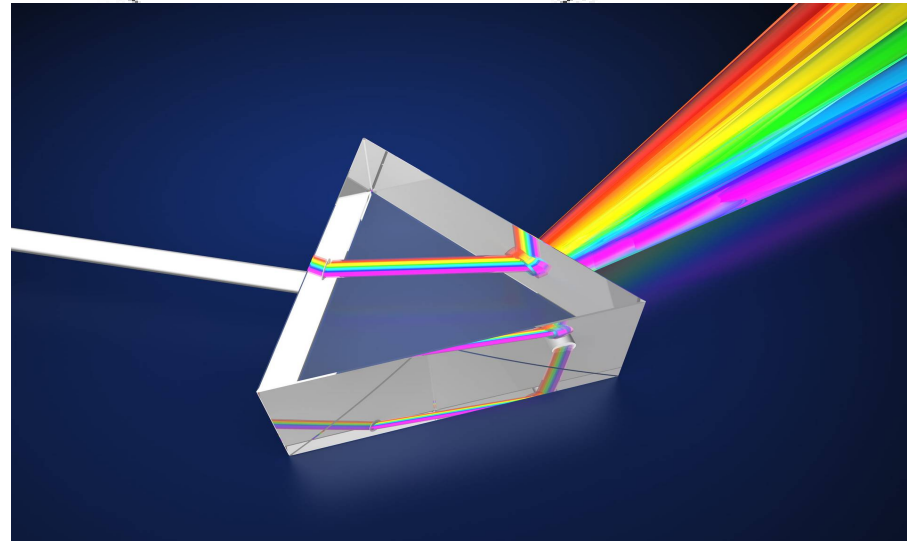
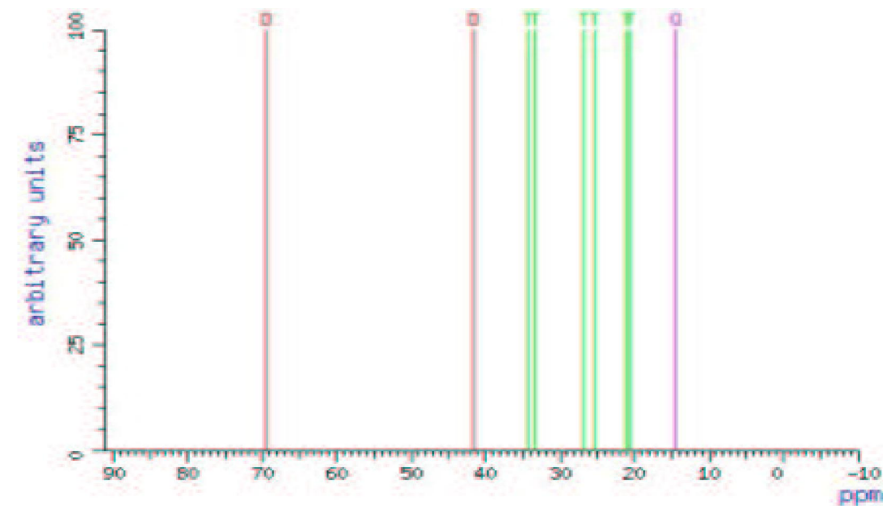
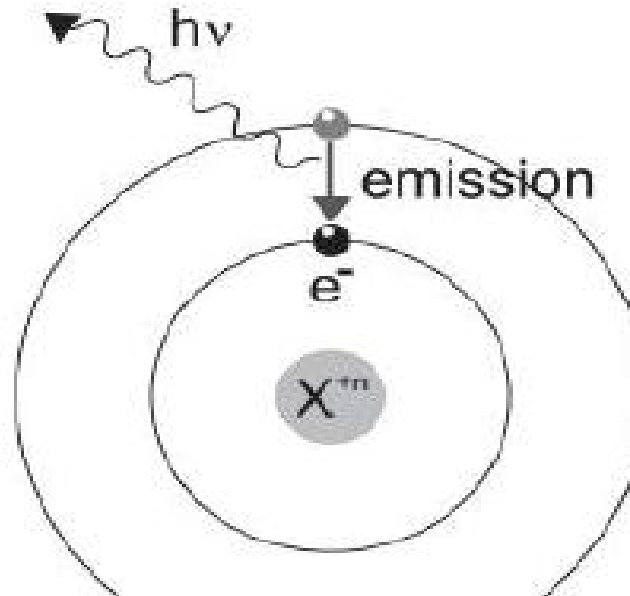
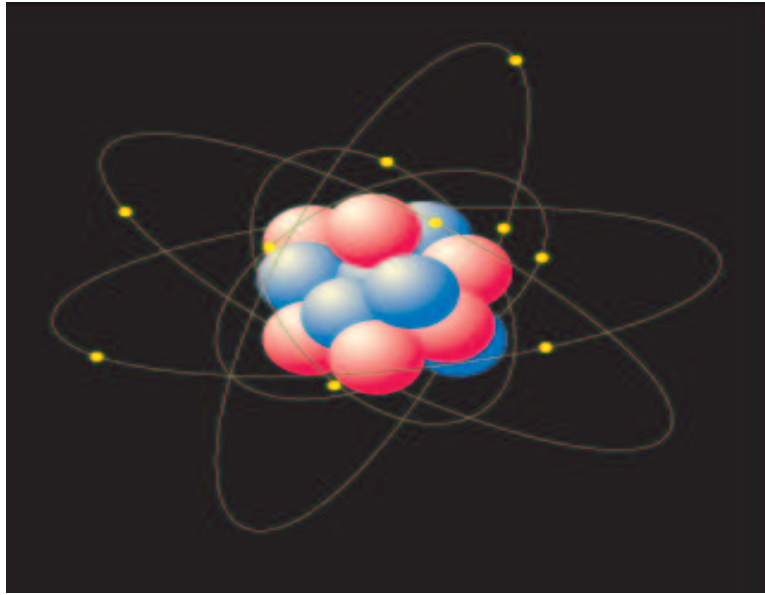


- Opacity $\kappa(\nu)$ is a fundamental quantity for radiation absorption during transmission in plasmas. Microscopically monochromatic opacity $\kappa(\nu)$ depends on two radiative processes:

1. Photoexcitation - $X^+Z + h\nu \rightarrow X^+Z^*$
2. Photoionization - $X^+Z + h\nu \rightarrow X^+Z^{+1} + e$

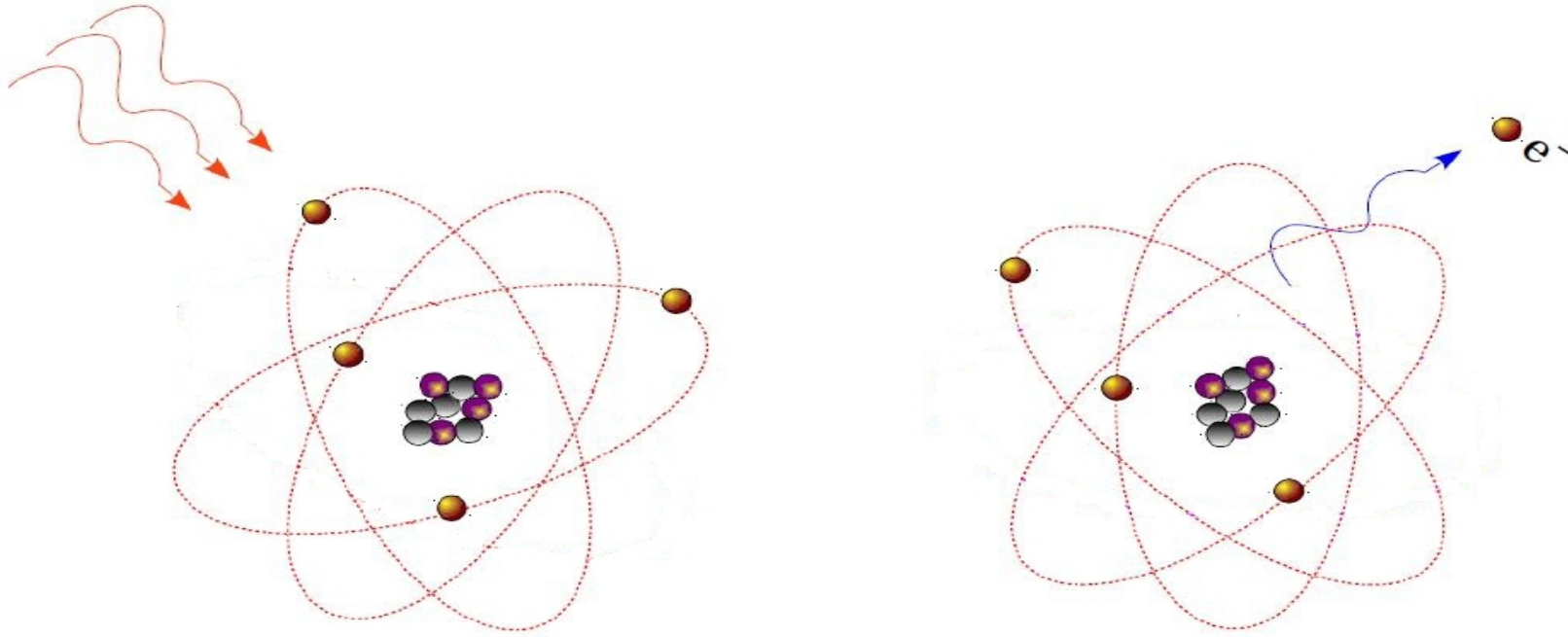
- **DIFFICULTY** - needs huge amount of atomic data: **The total $\kappa(\nu)$ is obtained from summed contributions of all possible transitions, both bound-bound & bound-continuum, from all ionization stages of all elements in the source**

ATOMS: THE UNDERLYING SCIENCE OF RADIATION



- Energy levels are quantized.
- An electron can be excited to higher levels. While dropping down, it gives out a photon. Radiation contains photons of many energies.
- SPECTRUM: Splitting the radiation in to its colors: Opacity - radiation absorption in transfer light it up a

Opacity: PHOTOIONIZATION (PI):



i) Direct Photoionization (background):



ii) **Resonant Photoionization:** an intermediate state before ionization $\rightarrow$ "Autoionizing state" $\rightarrow$ Resonant lines

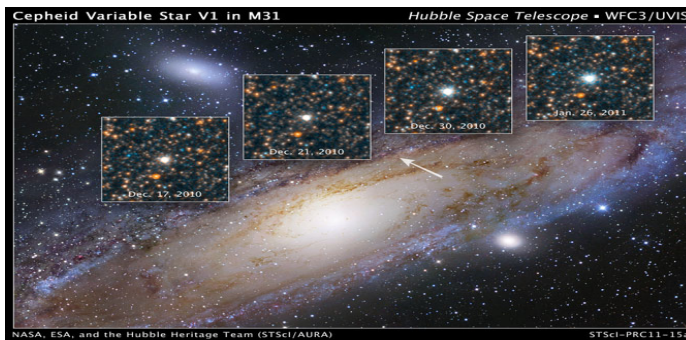


- κ_ν depends on photoionization cross section σ_{PI}

$$\kappa_\nu = N_{\text{i}} \sigma_{\text{PI}}(\nu)$$

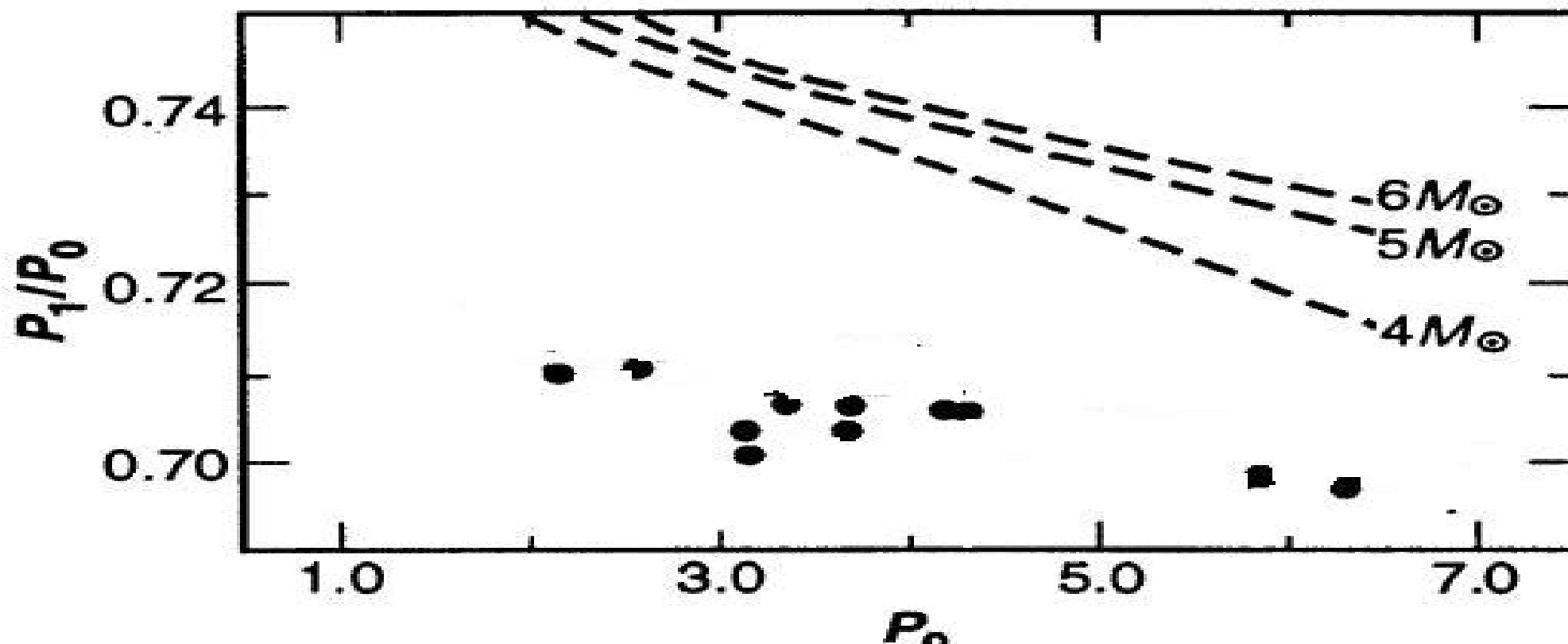


The OPACITY Project



The IRON Project

- **Cepheid are stars**, larger than the Sun, and go through periodic brightness and dimming states which can last for days to months
 - Luminosity (M_v) is proportional to the mass and opacity
- Discrepancy in predicted pulsation periods of Cepheid stars - REQUIRED HIGHER METALICITY/ OPACITY**

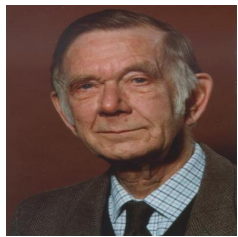


The OPACITY Project (OP) & The IRON Project (IP)

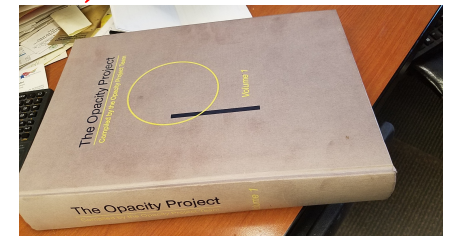
AIM: • Accurate Study of Atomic systems and process in astrophysical plasmas, • Obtain plasma opacities, • Applications to astrophysical problems

Needed: i) Development of Theory, ii) package of computer programs, and iii) a large team of scientists

• **THE OPACITY PROJECT (OP) (1983 - 2007, 2007 -):**



Prof. M.J. Seaton (1923 - 2007), UCL, UK



• The OP initiated and led by Seaton, - OP led to

• **THE IRON PROJECT (IP) (1991 -)**

CONTRIBUTORS: M.J. Seaton, W. Eissner, N. Badnell, M. Bautista, K.A. Berrington, AM Binello, P. Burke, V.M. Burke, K. Butler, G.X. Chen, MC Chidichimo, F. Delahaye, M Le Dourneuf, J.A. Fernley, M.E. Galavis, M Graziani, A. Hibbert, D.G. Hummer, A.E. Kingston, R Kisielius, D.J. Lennon, D. Luo, AE Lynas-Gray, H.E. Mason, M Melendez, C. Mendoza, D. Mihalas, M. Montenegro, **S.N. Nahar**, H. Nausbaumer, S Nakazaki, P. H. Norrington, P. Palmeri, G. Peach, J Pelan, A.K. Pradhan, P. Quinet, P Romano, H.P. Saraph, J.A. Tully, MC Witthoeft, Y. Yan, PR Young, C.J. Zeippen, V Zeman, G. Del Zenna, H.L. Zhang (52 authros)

New Physics:

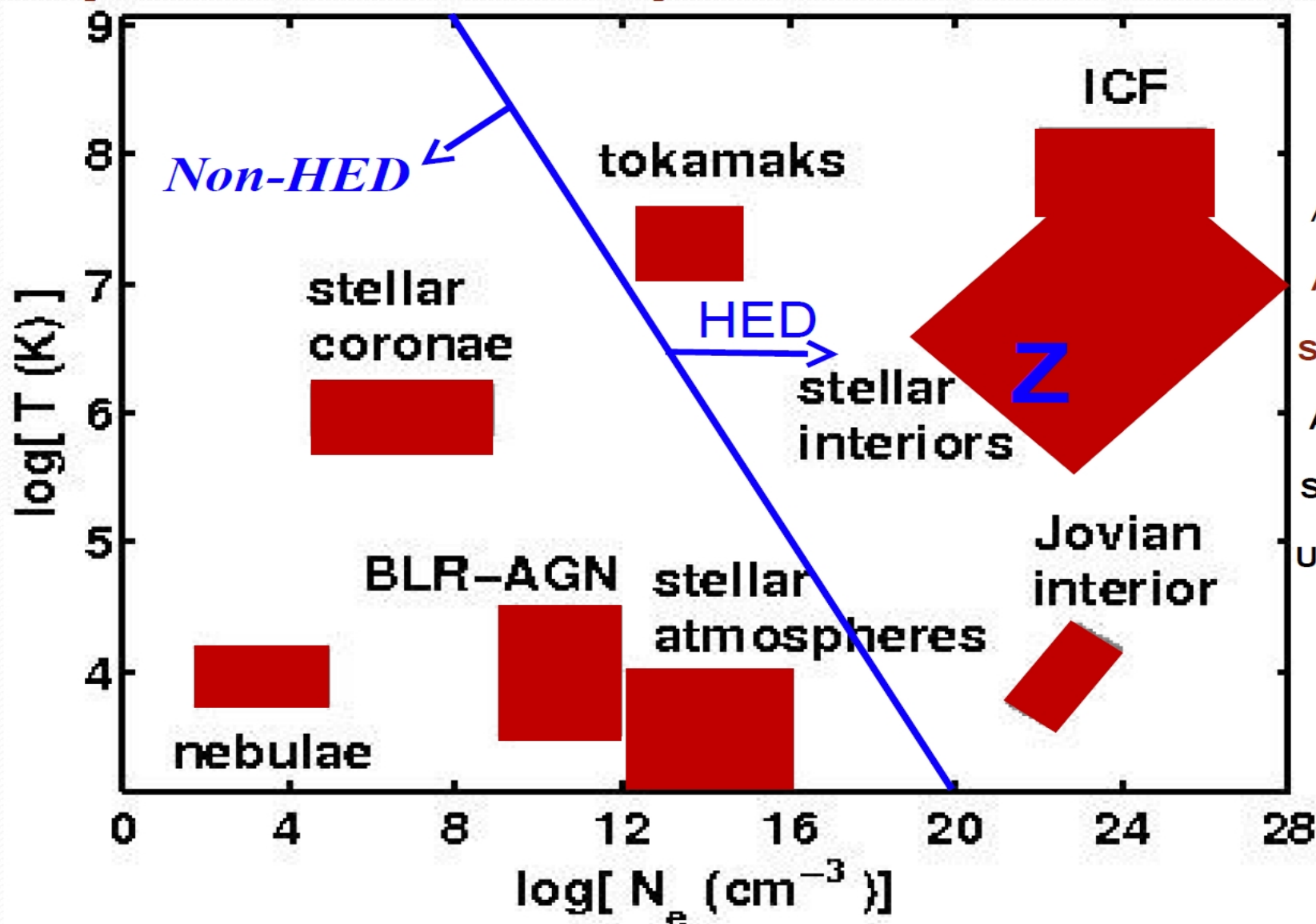
- Solved many astrophysical problems
- Found new physics in photoionization - features & X-ray lines
- Unified method for electron-ion was introduced
- High precision radiative and collisional data for applications
- Found new applications in nanobiomedicine

Publications:

- The Opacity Project (TOP) series: 22 papers in JPB,
- The Iron Project (TIP) series: 68 in A&A + additional ones outside
- Book chapters, conference conference proceedings articles
- Book: **The Opacity Project**, The Opacity Project team, IOP (1995)
- Textbook: "**Atomic Astrophysics and Spectroscopy**" (A.K. Pradhan & S.N. Nahar, Cambridge University press, 2011)
- **Atomic & Opacity Databases**
- **TOPbase (OP)** at CDS: <http://vizier.u-strasbg.fr/topbase/topbase.html>
 - Energy levels, Oscillator Strengths, Photoionization Cross Sections
- **TIPbase (IP)** at CDS: <http://cdsweb.u-strasbg.fr/tipbase/home.html>
 - Collisional Strengths for Electron Impact Excitations, and for Radiative Processes similar to TOPbase (not complete)
- **OPserver** for monochromatic opacities and program for mixtures at the OSC: <http://opacities.osc.edu/>
- **NORAD-Atomic-Data** at OSU: Latest radiative and electron-ion recombination data, <http://norad.astronomy.ohio-state.edu>

PLASMA COVERS 99% OF REGION IN T - ρ PHASE SPACE

Temperature-Density In HED Environments



Adapted From
“Atomic
Astrophysics
And
Spectroscopy”

Anil Pradhan
and
Sultana Nahar,
(Cambridge
University Press
2011)

- BLR-AGN (broad-line regions in active galactic nuclei), where many spectral features are associated with the central massive black hole
- Laboratory plasmas - tokamaks (magnetic confinement fusion devices), Z-pinch machines (inertial confinement fusion (ICF) devices)

Electron & Photon Distribution Functions in Plasmas

- The universe has largely charged particles and photons
- Temperature 'T' is defined differently for a radiation (photon) or the particle (electron)

$$E = h\nu \sim kT, \text{ or } E = 1/2mv^2 = 3/2kT$$

- Example: Consider a star ionizing a molecular cloud into a gaseous nebula - These two objects, the star & the nebula, have different T distribution functions
- A plasma of charged particles and a radiation field of photons is treated with two distribution functions, Planck (for photons) and Maxwell (for electrons)

PLANCK DISTRIBUTION FUNCTION FOR PHOTONS

- Energy of the radiation emitted by a black body, e.g. a star, is described by the Planck distribution function

$$B_\nu(T_*) = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT_*) - 1}, \quad (1)$$

T_* = radiation temperature, ν = frequency of the photons.

- Integrating $B_\nu(T_*)$ over the frequency, the radiance or energy per m^2sec emitted by an object at temperature T is given by Stefan-Boltzmann Law,

$$E = \sigma T^4 \quad (2)$$

$\sigma = 5.67 \times 10^{-8} \text{ Watts}/(\text{m}^2 \text{ K}^4) = \text{Stefan constant}$

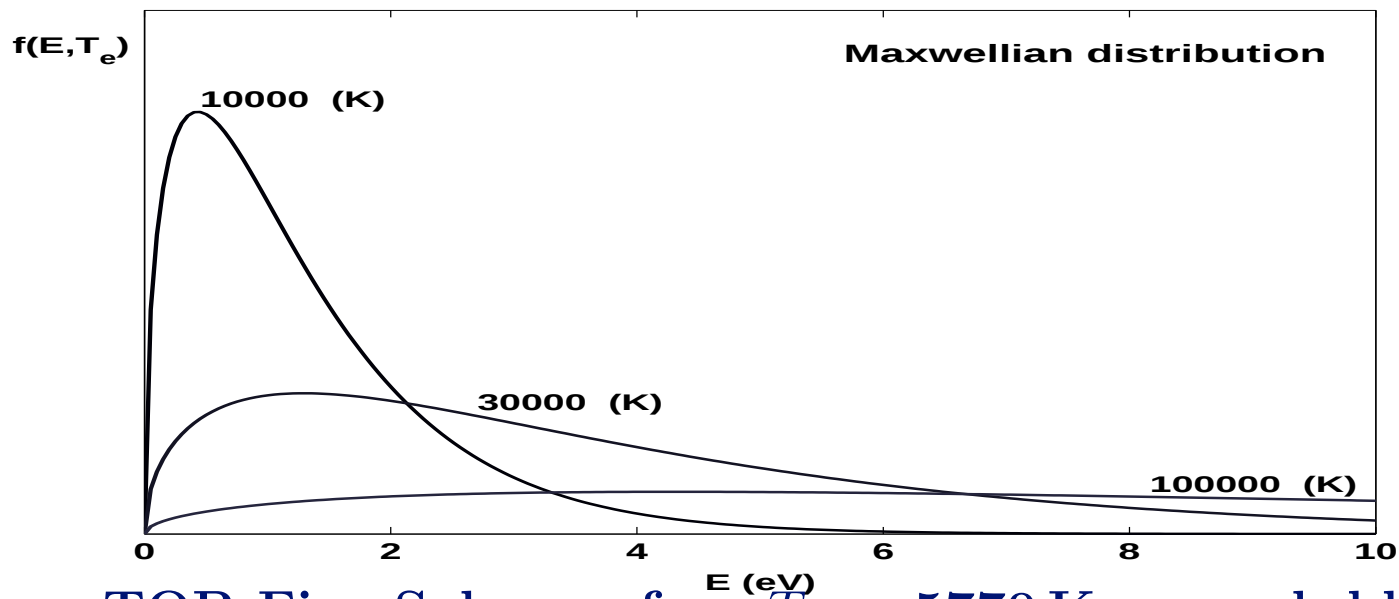
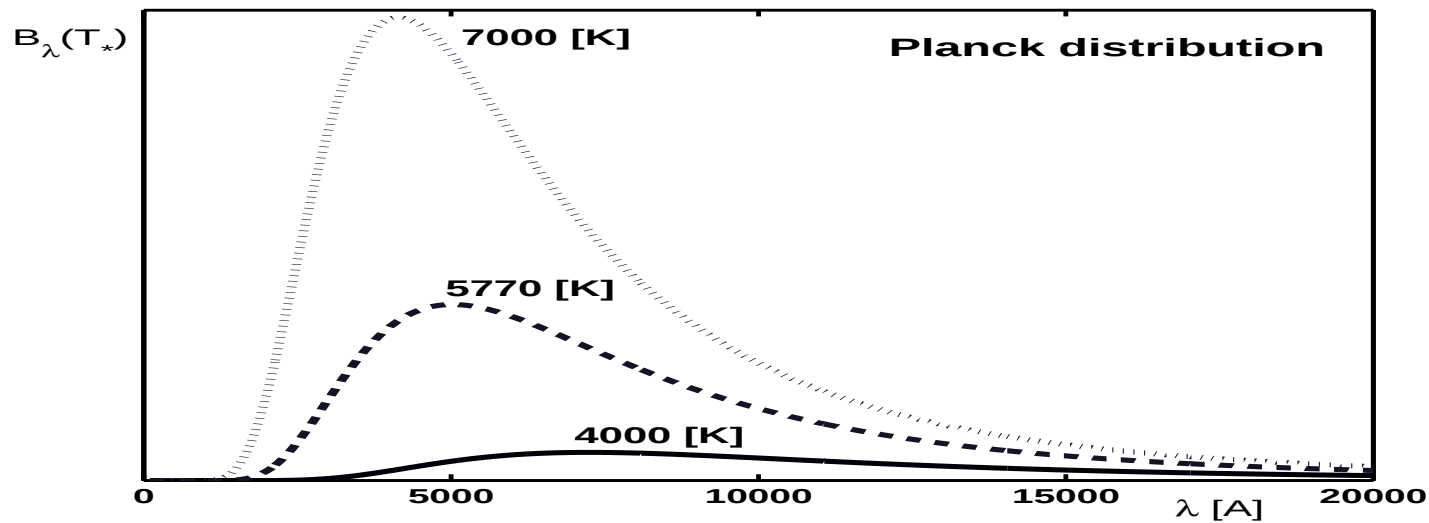
MAXWELL DISTRIBUTION FUNCTION FOR ELECTRONS

- Energy or velocity of charged particles (electrons) in the plasma ionized or heated by a star, e.g. in an H $\sim$ II region at temperature T is described by the Maxwell distribution function

$$f(\mathbf{v}) = \frac{4}{\sqrt{\pi}} \left(\frac{m}{2kT} \right)^{3/2} v^2 \exp \left(-\frac{mv^2}{2kT} \right). \quad (3)$$

- Distribution functions describe the energy behaviors of the ensemble of photons and electrons. They are needed for astrophysical modelings, such as, computing the rate coefficients of the atomic processes.

PLANCK & MAXWELL DISTRIBUTION FUNCTIONS



- TOP Fig: Solar surface $T_* = 5770 \text{ K} \rightarrow$ peak black body emission - yellow $\sim 5500 \text{ \AA}$.
- Bottom Fig: H II region (nebula): Ionized by star black body radiation of $T \sim 30000 - 40000 \text{ K}$, electron KE of Maxwellian distribution - $T_e \approx 10000 - 20000 \text{ K}$

Atomic Structure: CONSTITUENTS OF MATTER CREATED BY STARS

PERIODIC TABLE																		
Atomic Properties of the Elements																		
NIST National Institute of Standards and Technology U.S. Department of Commerce																		
Physical Measurement Laboratory www.nist.gov/pml																		
Standard Reference Data www.nist.gov/srd																		
Frequently used fundamental physical constants																		
For the most accurate values of these and other constants, visit physics.nist.gov/constants																		
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs																		
speed of light in vacuum c 299 792 458 m s ⁻¹ (exact)																		
Planck constant h 6,626 07 × 10 ⁻³⁴ J s ($h = h/2\pi$)																		
elementary charge e 1.602 177 × 10 ⁻¹⁹ C																		
electron mass m_e 9.109 38 × 10 ⁻³¹ kg																		
$m_e c^2$ 0.510 999 MeV																		
proton mass m_p 1.672 622 × 10 ⁻²⁷ kg																		
fine-structure constant α 1/137.035 999																		
Rydberg constant R_∞ 1.097 373 1569 m ⁻¹																		
$R_\infty c$ 3.289 841 960 × 10 ¹⁵ Hz																		
$R_\infty h c$ 13.605 69 eV																		
Boltzmann constant k 1,380 6 × 10 ⁻²³ J K ⁻¹																		
Solids Liquids Gases Artificially Prepared																		
Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H Hydrogen 1.008 1s																	2 He Helium 4.002602 1s ²
2	3 Li Lithium 6.94 1s ² 2s	4 Be Beryllium 9.0121831 1s ² 2s ²																10 Ne Neon 20.1797 1s ² 2s ² 2p ⁶
3	11 Na Sodium 22.98976928 [Ne]3s	12 Mg Magnesium 24.305 [Ne]3s ²																18 Ar Argon 39.948 [Ne]3s ² 3p ⁶
4	19 K Potassium 39.0983 [Ar]4s	20 Ca Calcium 40.078 [Ar]4s	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII	10 VIII	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
5	37 Rb Rubidium 85.4678 [Kr]5s	38 Sr Strontium 87.62 [Kr]5s ²	39 Y Yttrium 88.90584 [Kr]4d ¹ 5s ²	40 Zr Zirconium 91.224 [Kr]4d ² 5s ²	41 Nb Niobium 92.90637 [Kr]4d ⁴ 5s ²	42 Mo Molybdenum 95.95 [Kr]4d ⁵ 5s ¹	43 Tc Technetium (98) [Kr]4d ⁵ 5s ²	44 Ru Ruthenium 101.07 [Kr]4d ⁶ 5s ¹	45 Rh Rhodium 102.90550 [Kr]4d ⁷ 5s ¹	46 Pd Palladium 106.42 [Kr]4d ¹⁰	47 Ag Silver 107.8682 [Kr]4d ¹⁰ 5s ¹	48 Cd Cadmium 112.414 [Kr]4d ¹⁰ 5s ²	49 In Indium 114.818 [Kr]4d ¹⁰ 5s ² 5p ¹	50 Sn Tin 118.710 [Kr]4d ¹⁰ 5s ² 5p ²	51 Sb Antimony 121.760 [Kr]4d ¹⁰ 5s ² 5p ³	52 Te Tellurium 127.60 [Kr]4d ¹⁰ 5s ² 5p ⁴	53 I Iodine 126.90447 [Kr]4d ¹⁰ 5s ² 5p ⁵	54 Xe Xenon 131.293 [Kr]4d ¹⁰ 5s ² 5p ⁶
6	55 Cs Cesium 132.9054520 [Xe]6s	56 Ba Barium 137.327 [Xe]6s ²		72 Hf Hafnium 178.49 [Xe]4f ¹⁴ 5d ² 6s ²	73 Ta Tantalum 180.94788 [Xe]4f ¹⁴ 5d ³ 6s ²	74 W Tungsten 183.84 [Xe]4f ¹⁴ 5d ⁴ 6s ²	75 Re Rhenium 186.207 [Xe]4f ¹⁴ 5d ⁵ 6s ²	76 Os Osmium 190.23 [Xe]4f ¹⁴ 5d ⁶ 6s ²	77 Ir Iridium 192.217 [Xe]4f ¹⁴ 5d ⁷ 6s ²	78 Pt Platinum 195.084 [Xe]4f ¹⁴ 5d ⁹ 6s ¹	79 Au Gold 196.966569 [Xe]4f ¹⁴ 5d ¹⁰ 6s ¹	80 Hg Mercury 200.592 [Xe]4f ¹⁴ 5d ¹⁰ 6s ²	81 Tl Thallium 204.38 [Hg]6p ¹	82 Pb Lead 207.2 [Hg]6p ²	83 Bi Bismuth 208.98040 [Hg]6p ³	84 Po Polonium (209) [Hg]6p ⁴	85 At Astatine (210) [Hg]6p ⁵	86 Rn Radon (222) [Hg]6p ⁶
7	87 Fr Francium (223) [Rn]7s	88 Ra Radium (226) [Rn]7s ²		104 Rf Rutherfordium (267) [Rn]5f ¹⁴ 6d ² 7s ²	105 Db Dubnium (268) [Rn]5f ¹⁴ 6d ³ 7s ²	106 Sg Seaborgium (271) [Rn]5f ¹⁴ 6d ⁴ 7s ²	107 Bh Bohrium (272) [Rn]5f ¹⁴ 6d ⁵ 7s ²	108 Hs Hassium (270) [Rn]5f ¹⁴ 6d ⁶ 7s ²	109 Mt Meitnerium (276) [Rn]5f ¹⁴ 6d ⁷ 7s ²	110 Ds Darmstadtium (281) [Rn]5f ¹⁴ 6d ⁸ 7s ²	111 Rg Roentgenium (280) [Rn]5f ¹⁴ 6d ⁹ 7s ²	112 Cn Copernicium (285) [Rn]5f ¹⁴ 6d ¹⁰ 7s ²	113 Uut Ununtrium (284) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ¹	114 Fl Flerovium (289) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ²	115 Uup Ununpentium (288) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ³	116 Lv Livermorium (293) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁴	117 Uus Ununseptium (294) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁵	118 Uuo Ununoctium (294) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁶
			Lanthanides	57 La Lanthanum 138.90547 [Xe]5d ¹ 6s ²	58 Ce Cerium 140.116 [Xe]4f ¹ 5d ¹ 6s ²	59 Pr Praseodymium 140.907 [Xe]4f ² 6s ²	60 Nd Neodymium 144.242 [Xe]4f ³ 6s ²	61 Pm Promethium (145) [Xe]4f ⁴ 6s ²	62 Sm Samarium 150.36 [Xe]4f ⁵ 6s ²	63 Eu Europium 151.964 [Xe]4f ⁶ 6s ²	64 Gd Gadolinium 157.25 [Xe]4f ⁷ 5d ¹ 6s ²	65 Tb Terbium 158.92535 [Xe]4f ⁸ 6s ²	66 Dy Dysprosium 162.500 [Xe]4f ⁹ 6s ²	67 Ho Holmium 164.93033 [Xe]4f ¹⁰ 6s ²	68 Er Erbium 167.259 [Xe]4f ¹¹ 6s ²	69 Tm Thulium 168.93422 [Xe]4f ¹² 6s ²	70 Yb Ytterbium 173.054 [Xe]4f ¹³ 6s ²	71 Lu Lutetium 174.9668 [Xe]4f ¹⁴ 5d ¹ 6s ²
			Actinides	89 Ac Actinium (227) [Rn]6d ¹ 7s ²	90 Th Thorium 232.0377 [Rn]6d ² 7s ²	91 Pa Protactinium 231.03588 [Rn]5f ¹ 6d ¹ 7s ²	92 U Uranium 238.02891 [Rn]5f ³ 6d ¹ 7s ²	93 Np Neptunium (237) [Rn]5f ⁴ 6d ¹ 7s ²	94 Pu Plutonium (244) [Rn]5f ⁶ 7s ²	95 Am Americium (243) [Rn]5f ⁷ 7s ²	96 Cm Curium (247) [Rn]5f ⁸ 6d ¹ 7s ²	97 Bk Berkelium (247) [Rn]5f ⁹ 7s ²	98 Cf Californium (251) [Rn]5f ¹⁰ 7s ²	99 Es Einsteinium (252) [Rn]5f ¹¹ 7s ²	100 Fm Fermium (257) [Rn]5f ¹² 7s ²	101 Md Mendelevium (258) [Rn]5f ¹³ 7s ²	102 No Nobelium (259) [Rn]5f ¹⁴ 7s ²	103 Lr Lawrencium (262) [Rn]5f ¹⁴ 7s ² 7p ¹

Atomic Number

Ground-state Level

Symbol

Name

Standard Atomic Weight†

Ground-state Configuration

Ionization Energy (eV)

†Based upon ¹²C. () indicates the mass number of the longest-lived isotope.

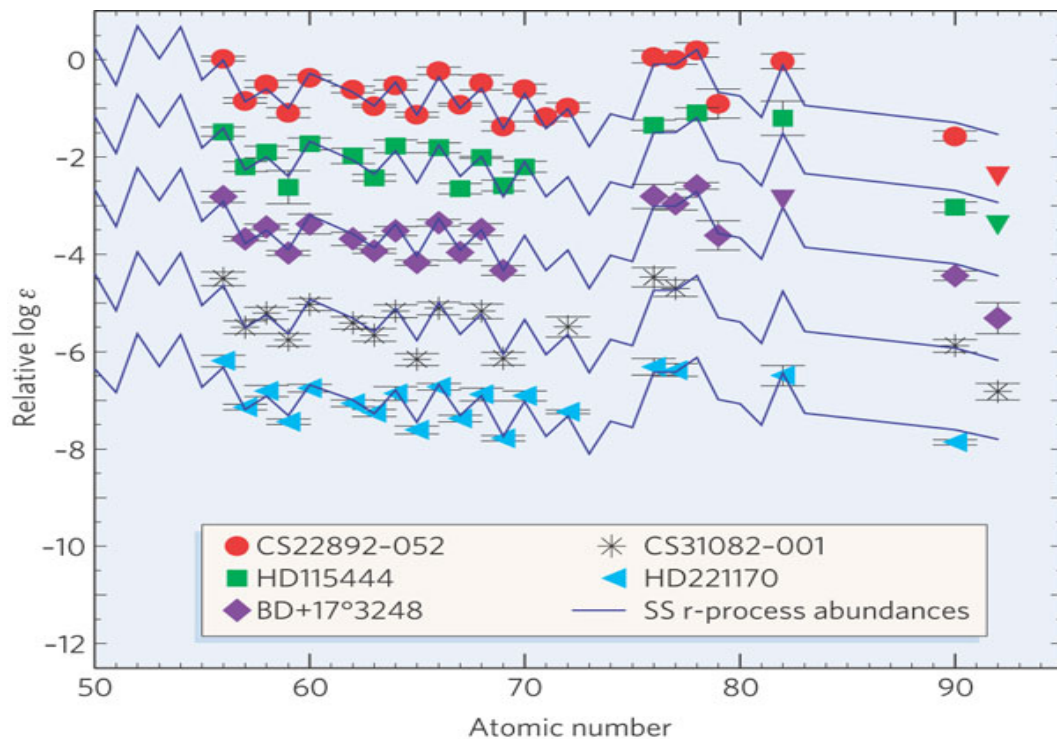
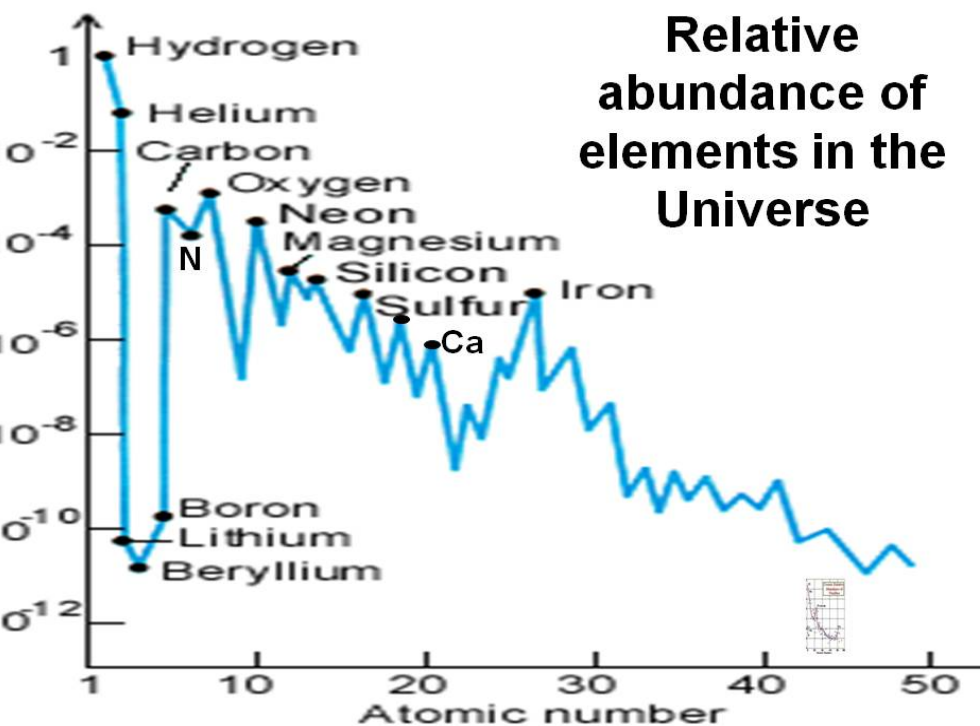
*IUPAC conventional atomic weights; standard atomic weights for these elements are expressed in intervals; see iupac.org for an explanation and values.

For a description of the data, visit physics.nist.gov/data

NIST SP 966 (September 2014)

- Elements: Gases (pink), Solids (white), Liquids (blue). A lab generated yellow element is replaced with astrophysical observation
- Elements are created through nuclear fusion. It starts with creating He from 2 H atoms. As plasma density and T increase in the stellar core, Li, C, N, O etc are created, and the process continues up to **Fe**

ABUNDANCES OF HEAVY ELEMENTS IN SPACE



- Nuclear fusion cycle in a star ends at Fe (strongest nuclear force). Elemental abundances go down beyond Fe. **Fortunate to have elemental abundances on the Earth. Solar system was made from debris of supernova explosions**
- Heavy elements are created through neutron capture - s-process in the star and r-process during supernova explosions **New! Kilonova - mergers of black holes and neutron stars**
- Metals, only with 3%, provide the maximum information
- 99% of the matter exist in the plasma state

STUDYING ASTRONOMICAL OBJECTS

- 99% of known matter is plasma

ASTRONOMICAL objects are studied in three ways:

- **IMAGING:**

- Beautiful pictures of astronomical objects, Stars, Nebulae, Active Galactic Nuclei, Black hole Environments, etc
→ Provides information of size and location of the objects

- **PHOTOMETRY:**

- Low resolution spectroscopy - Bands of Electromagnetic Colors ranging from X-ray to Radio waves
→ macroscopic information

- **SPECTROSCOPY:**

- Taken by spectrometer - Provides most of the detailed knowledge: temperature, density, extent, chemical composition, etc. of astronomical objects

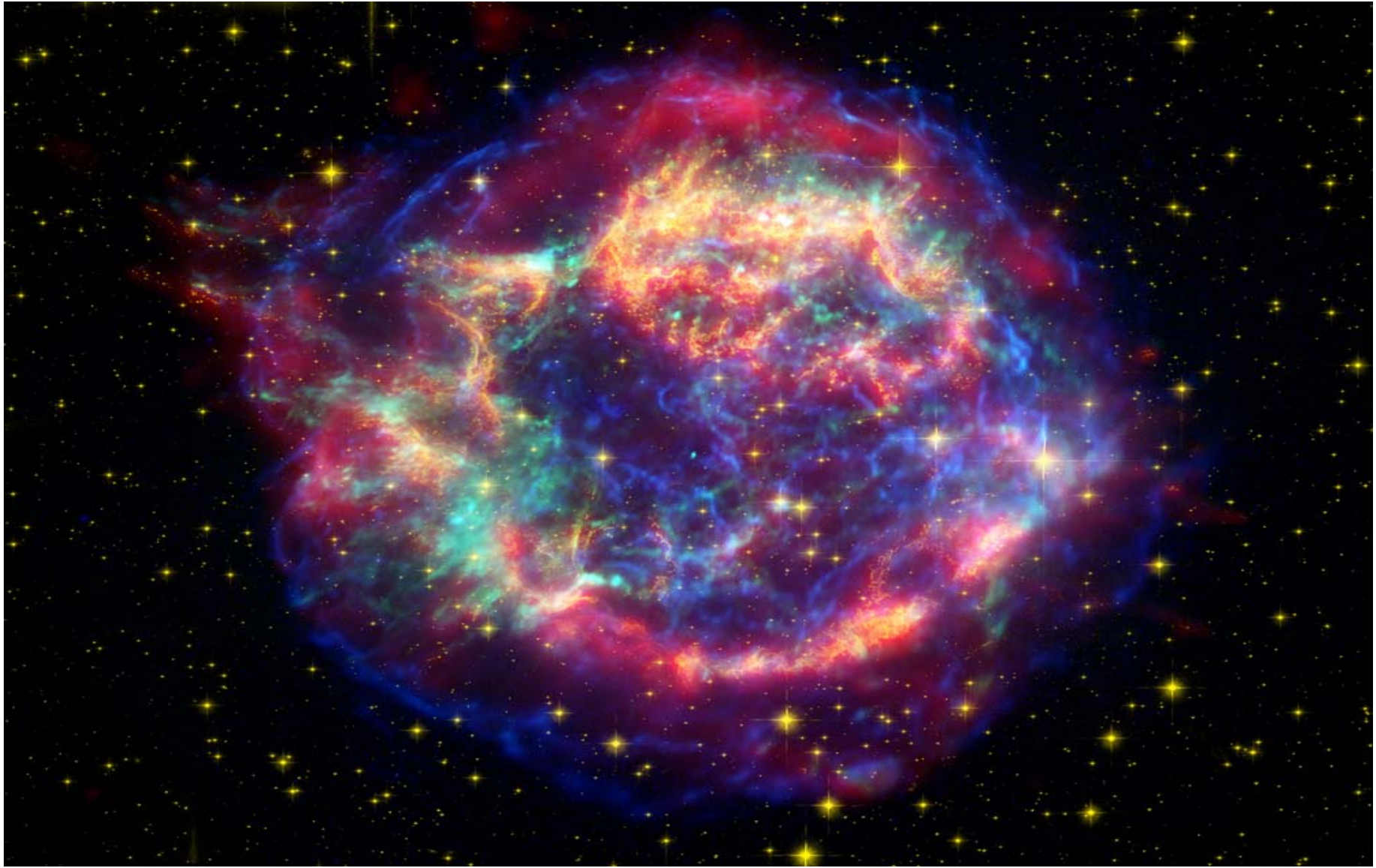
Spectroscopy is underpinned by Atomic & Molecular Physics

ETA CARINAE: IMAGE



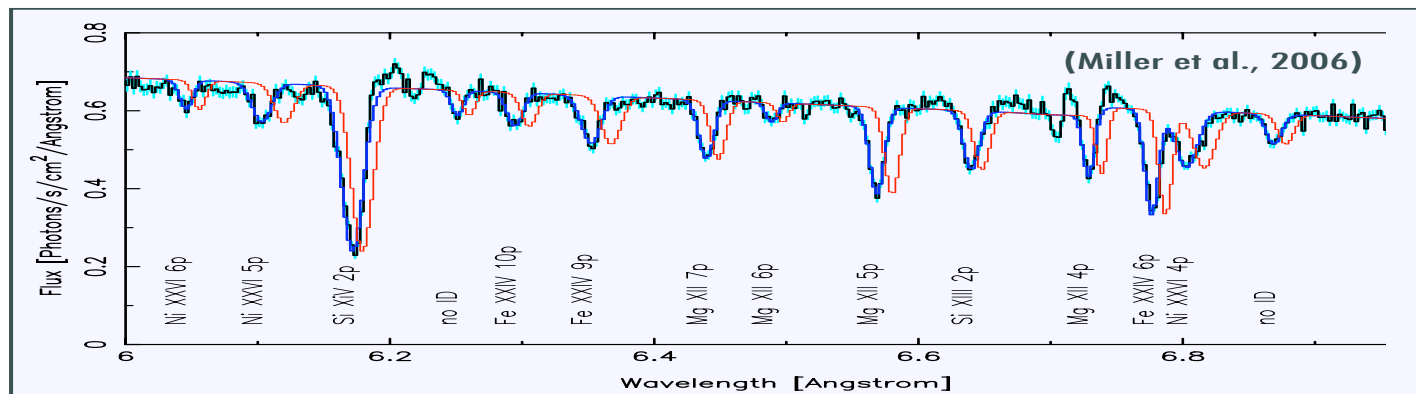
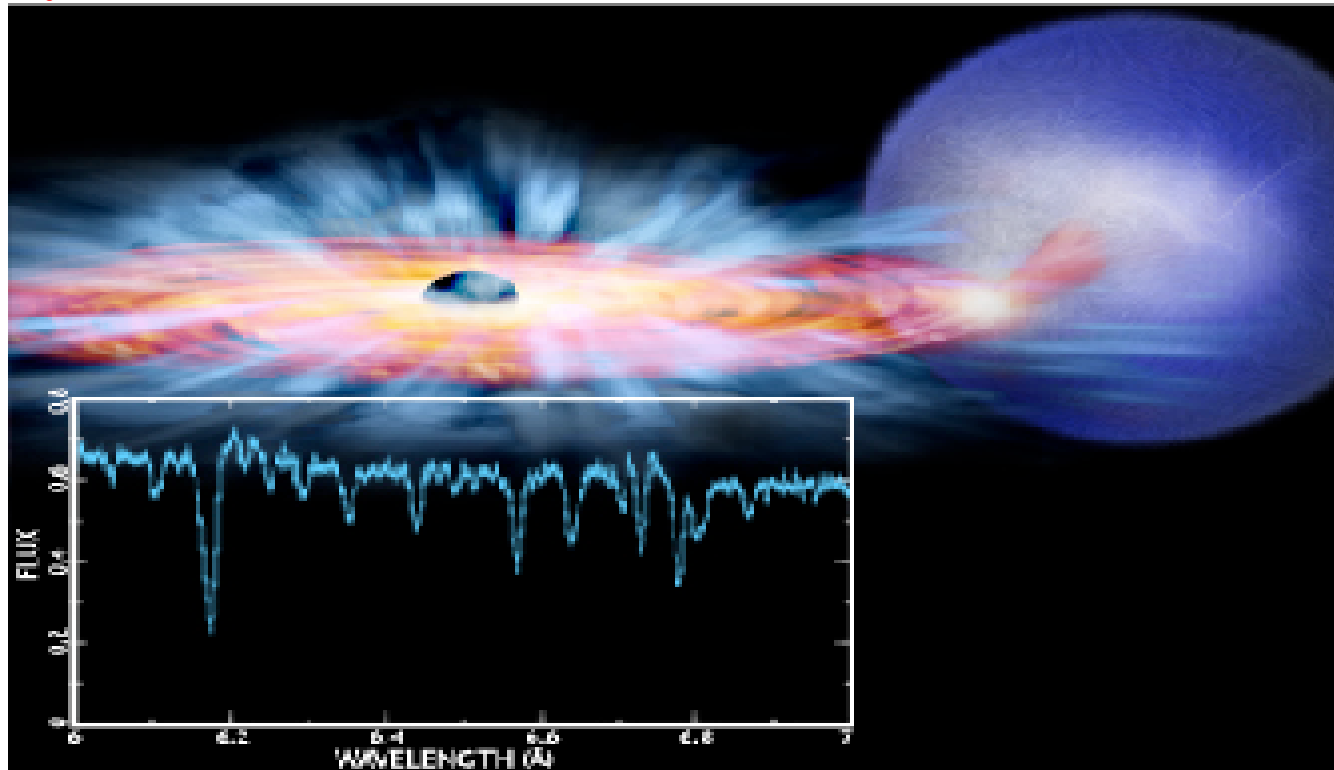
- Consists of 2 massive bright (5M times the sun) stars, heavier one went under a near supernova explosion
- Explosion produced two polar lobes, and a large but thin equatorial disk, all moving outward at 670 km/s. Mass indicates future eruptions
- HST image shows the bipolar Homunculus Nebula around it

SUPERNOVA REMNANT CASSIOPEIA A: PHOTOMETRIC



- Heavier elements: r (rapid)-process during Supernova explosion
- Solar system made from debris of supernova explosions

SPECTRUM of the Wind near Black hole: GRO J1655-40 Binary Star System

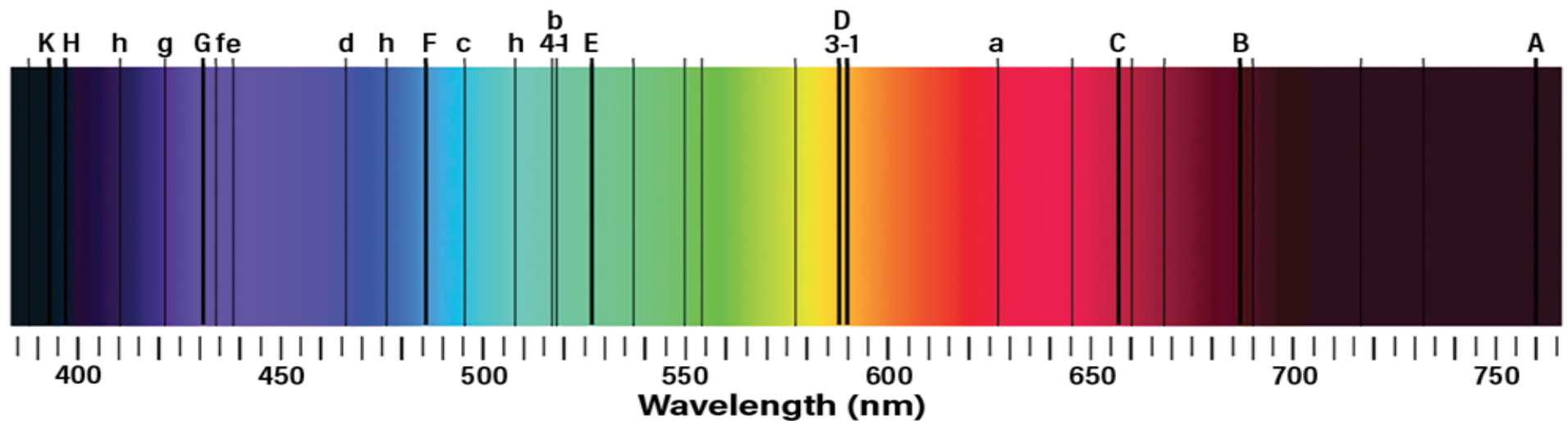


- Materials from the large star is sucked into companion black hole - form wind as they spiral to it. Spectrum of the wind (BLUE):
- Highly charged Mg, Si, Fe, Ni lines. RED: Elements in natural widths
- Doppler Blue Shift - Wind is blowing toward us

SOLAR SPECTRA: Need for QUANTUM MECHANICS

- Absorption line - forms as an electron absorbs a photon to jump to a higher energy level - seen above the continuum background
- Emission line - forms as a photon is emitted due to the electron dropping to a lower energy level - seen below the continuum
- For the same transition levels, lines form at the same energy position

THE SUN'S SPECTRUM



- Fraunhofer (1815) observed lines in the solar spectrum & used alphabet for designation
- Later spectroscopy with quantum mechanics identified them: A (7594 Å, O), B (6867 Å, O) (air), C (6563 Å H), D1 & D2 (5896, 5890 Å Na, yellow sun), E (5270 Å, Fe I), F (4861 Å, H), G (4300 Å, CH), H & K (3968, 3934 Å, Ca II)
- Russel and Saunders (1925) introduced LS coupling designation

ATOMIC STRUCTURE

- Atomic structure - i) Organization of electrons in various shells and subshells, ii) Determinations of electron energies and wave functions
- As Fermions, unlike Bosons, electrons form *structured* arrangements bound by the attractive nuclear potential
- Different atomic states arise from quantization of motion, orbital and spin angular momenta of all electrons. Transitions among those states involve photons which are seen as lines in observed spectra
- The combination of orbital angular momentum L and spin angular momentum S follow strict coupling rules, known as **selection rules**, that determine the stationary energy states and expectation values, such as, mean radius.
- The dynamic state of an atom - described by a Schrodinger equation
- HYDROGEN ATOM - only atomic system that can be treated exactly
- **Approximation begins from 2-electrons systems**

HYDROGEN ATOM

Schrodinger equation of hydrogen, with $\text{KE} = \mathbf{P}^2/(2m)$ and nuclear potential energy $V(\mathbf{r})$, is

$$\left[-\frac{\hbar^2}{2m} (\nabla^2) + V(r) \right] \Psi = E \Psi \quad (4)$$

or,

$$\left[-\frac{\hbar^2}{2m} (\nabla_r^2 + \nabla_\perp^2) + V(r) \right] \Psi = E \Psi$$
$$V(r) = -\frac{Ze^2}{r} = -\frac{2Z}{r/a_0} \text{Ry}$$

In spherical coordinates

$$\nabla_{\mathbf{r}}^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \quad (5)$$
$$\nabla_\perp^2 = \frac{1}{r^2 \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial}{\partial \vartheta} \right) + \frac{1}{r^2 \sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2}$$

The solution or wavefunction has independent variables r , θ , ϕ , each will correspond to a quantum number,

$$\Psi(\mathbf{r}, \vartheta, \varphi) = R(r) Y(\vartheta, \varphi)$$

ANGULAR EQUATION & m QUANTUM NUMBER

The angular equation is separated with constant λ as

$$\frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial \mathbf{Y}}{\partial \vartheta} \right) + \frac{1}{\sin^2 \vartheta} \frac{\partial^2 \mathbf{Y}}{\partial \phi^2} + \lambda \mathbf{Y} = 0 \quad (6)$$

The solutions are spherical harmonics,

$$\mathbf{Y}(\vartheta, \varphi) = \Theta(\vartheta) \Phi(\varphi) \quad (7)$$

The equation can be expressed in the form

$$\mathbf{L}^2 \mathbf{Y}(\vartheta, \varphi) = \left[-\frac{\hbar^2}{2m} (\nabla^2) \right] \mathbf{Y}(\vartheta, \varphi) = \lambda \mathbf{Y}(\vartheta, \varphi), \quad (8)$$

L is an angular momentum operator. Substituting Y ,

$$\frac{d^2 \Phi}{d\varphi^2} + \nu \Phi = 0, \quad (9)$$
$$\frac{1}{\sin \vartheta} \frac{d}{d\vartheta} \left(\sin \vartheta \frac{d\Theta}{d\vartheta} \right) + \left(\lambda - \frac{\nu}{\sin^2 \vartheta} \right) \Theta = 0,$$

where $\nu = m^2$, and $\Phi(\varphi) = (2\pi)^{-1/2} e^{im\varphi}$. m = *magnetic angular quantum number* and equals to $0, \pm 1, \pm 2, \dots$

ANGULAR EQUATION & 1 QUANTUM NUMBER

Replacing ϑ by $w = \cos \vartheta$ the Θ equation is

$$\frac{d}{dw} \left[(1 - w^2) \frac{d\Theta}{dw} \right] + \left[\lambda - \frac{m^2}{1 - w^2} \right] \Theta(w) = 0. \quad (10)$$

A finite solution Θ requires $\lambda = l(l + 1)$, where $l = 0, 1, 2, \dots$. The solutions are associated Legendre polynomials of order l and m ,

$$P_l^m(w) = (1 - w^2)^{|m|/2} \frac{d^{|m|}}{dw^{|m|}} P_l(w), \quad (11)$$

$m = l, l - 1, \dots, -l$. $m = 0 \rightarrow P_l(w) =$ Legendre polynomial of order l . The angular solution of normalized spherical harmonic:

$$Y_{lm}(\vartheta, \varphi) = N_{lm} P_l^m(\cos \vartheta) e^{im\varphi} \quad (12)$$

where

$$N_{lm} = \epsilon \left[\frac{2l + 1}{4\pi} \frac{(l - |m|)!}{(l + |m|)!} \right]^{1/2}, \quad (13)$$

$\epsilon = (-1)^m$ for $m > 0$ and $\epsilon = 1$ for $m \leq 0$.

ANGULAR MOMENTUM OPERATOR

Spherical harmonics satisfy the orthogonality condition

$$\int_{\varphi=0}^{2\pi} \int_{\vartheta=0}^{\pi} Y_{l_1 m_1}^*(\vartheta, \varphi) Y_{l_2 m_2}(\vartheta, \varphi) \sin \vartheta \, d\vartheta \, d\varphi = \delta_{l_1, l_2} \delta_{m_1, m_2} \quad (14)$$

The equation with angular momentum operator can now be written as

$$L^2 Y_l^m(\vartheta, \varphi) = l(l+1) \hbar^2 Y_l^m(\vartheta, \varphi) \quad (15)$$

With angular momentum $L = mvr = m\omega r^2$ the angular frequency $\omega = L/mr^2$, the centripetal force is $m\omega^2 r = L^2/mr^3$ and the corresponding potential energy is

$$V_{\text{ang}} = \frac{1}{2} m \omega^2 r^2 = \frac{L^2}{2mr^2}. \quad (16)$$

This is similar to the second potential term of hydrogen provided

$$L^2 = l(l+1) \hbar^2; \quad (17)$$

THE RADIAL EQUATION

The radial equation representing the dynamical motion of the electron is

$$\left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{2m}{\hbar^2} \left(E - V(r) \right) - \frac{\lambda}{r^2} \right] R(r) = 0, \quad (18)$$

Substituting $R(r) = P(r)/r$, it is reduced to

$$\left[\frac{\hbar^2}{2m} \frac{d^2}{dr^2} - V(r) - \frac{l(l+1)\hbar^2}{2mr^2} + E \right] P(r) = 0. \quad (19)$$

The equation shows motion of a particle in a potential

$$V(r) + \frac{l(l+1)\hbar^2}{2mr^2}, \quad (20)$$

We switch to Rydberg unit for the Schrodinger equation,

$$\left[\frac{d^2}{d(r/a_0)^2} + \frac{2Z}{r/a_0} - \frac{l(l+1)}{(r/a_0)^2} + E/R_y \right] P(r) = 0 \quad (21)$$

$$\text{or, } \left[\frac{d^2}{dr^2} - V(r) - \frac{l(l+1)}{r^2} + E \right] P(r) = 0, \quad (22)$$

SOLVING RADIAL EQUATION

- The radial equation can be solved on specifying boundary conditions, (i) r at ∞ , and (ii) r near $r = 0$
- The bound electron moves in the nuclear attractive potential: $\lim_{r \rightarrow \infty} V(r) = 0$. Hence for case (i) for $r \rightarrow \infty$

$$\left[\frac{d^2}{dr^2} + E \right] P(r) = 0, \quad (23)$$

which has solutions

$$P(r) = e^{\pm ar}, \quad a = \sqrt{-E}. \quad (24)$$

Taking $E < 0$ for bound states, $\lim_{r \rightarrow \infty} e^{-ar}$ is a possible solution. It is also valid for $E > 0$, when a becomes imaginary. Hence, the asymptotic behavior suggests

$$P(r) = e^{-ar} f(r) \quad (25)$$

subject to $\lim_{r \rightarrow 0} f(r) = 0$. On substitution,

$$\frac{d^2 f}{dr^2} - 2a \frac{df}{dr} + \left[\frac{2Z}{r} - \frac{l(l+1)}{r^2} \right] f(r) = 0 \quad (26)$$

WAVEFUNCTION & n QUANTUM NUMBER

- For $r \ll 1$, the solution $f(r)$ is expressed as a power series

$$f(r) = r^s [A_0 + A_1 r + A_2 r^2 + \dots]$$

Finite f as $r \rightarrow 0$ requires $s > 0$ for consistent behavior of a bound electron. The possible radial wave function is

$$P(r) = f(r)e^{-ar} \approx r^{l+1}e^{-ar} \quad (27)$$

at large distances r . This again diverges at infinity, unless the series for f terminates at a point where the energy is

$$E = -(Z^2/n^2) \times Ry; \quad (28)$$

n is a positive integer & defined as the *principal quantum number*. Full $P(r)$ in Laguerre polynomial L is,

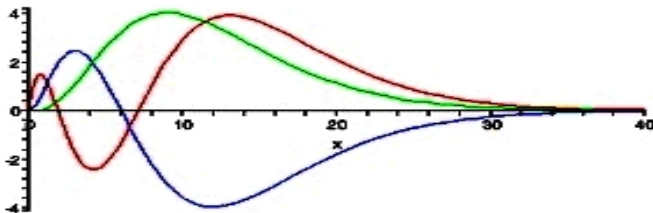
$$P_{nl}(r) = \sqrt{\frac{(n-l-1)!Z}{n^2[(n+l)!]^3 a_0}} \left[\frac{2Zr}{na_0} \right]^{l+1} e^{\frac{-Zr}{na_0}} \times L_{n+l}^{2l+1} \left(\frac{2Zr}{na_0} \right),$$

where

$$L_{n+l}^{2l+1}(\rho) = \sum_{k=0}^{n-l-1} \frac{(-1)^{k+2l+1} [(n+l)!]^2 \rho^k}{(n-l-1-k)!(2l+1+k)!k!}. \quad (29)$$

QUANTUM DESIGNATION OF A STATE

- Atomic Shells: $n = 1, 2, 3, 4 \dots = K, L, M, N$
- No of electrons = $2n^2$ - Closed shell, $< 2n^2$ - Open Shell
- Orbital angular momentum: $l = 0, 1, 2, 3, 4 \dots (n-1) = s, p, d, f, \dots$
- Total Angular Momentum: $L = 0, 1, 2, 3, 4, \dots, = S, P, D, F, \dots$
- Magnetic angular momentum: $m_l = 0, \pm 1, \pm 2, \pm 3, 4 \dots \pm l$
 $(2l+1)$ values $\rightarrow$ angular momentum multiplicity = $2L+1$
- Spin angular momentum S was introduced due to electron spin. It is inherent in Dirac equation. $S = \text{integer or } 1/2 \text{ integer depending on number of electrons with spin } s=1/2$
- Spin magnetic angular momentum = $m_s = \pm S$ - $(2S+1)$ values - spin multiplicity
- Spin multiplicity = $1, 2, 3, \dots = \text{singlet, doublet, triplet} \dots$
- Total angular momentum: $J = |L \pm S|$, $J_M = 0, \pm 1, \pm 2, \pm 3, 4 \dots \pm J$, J multiplicity = $2J + 1$
- Parity (introduced from wavefunction) = $\pi = (-1)^l = +1$ (even) or -1 (odd)
- Symmetry of a state: $(^{2S+1})L^\pi$ (LS), $(^{2S+1})L_J^\pi$ (LSJ - fine structure)
- No of nodes in a wavefunction = $n-l-1$



SPECTRAL LINES & RYDBERG FORMULA

Transition of states: Hydrogen spectral line - Photon emitted or absorbed is of energy (Rydberg formula)

$$\Delta\mathcal{E}_{n,n'} = \frac{1}{\lambda} = \mathcal{R}_H \left[\frac{1}{n^2} - \frac{1}{n'^2} \right] \quad (n' > n), \quad (30)$$

where $\mathcal{R}_H = 109,677.576 / \text{cm} = 1/911.76 / \text{\AA}$ is the Rydberg constant.
H ionization energy ($n=1, n' = \infty$) = $911.76 \text{ \AA} = 1 \text{ Ry} = 13.6 \text{ eV}$.
Energy in wavelength in Ångström units:

$$\lambda = \frac{911.76 \text{ \AA}}{\Delta E / \text{Ry}}. \quad (31)$$

• $\Delta\mathcal{E}_{n,n'}$ yields series of hydrogen spectral lines,

$$\mathcal{R}_H \left[1 - \frac{1}{n'^2} \right], \quad n' = 2, 3, 4, \dots \quad \text{Lyman (Ly)}$$

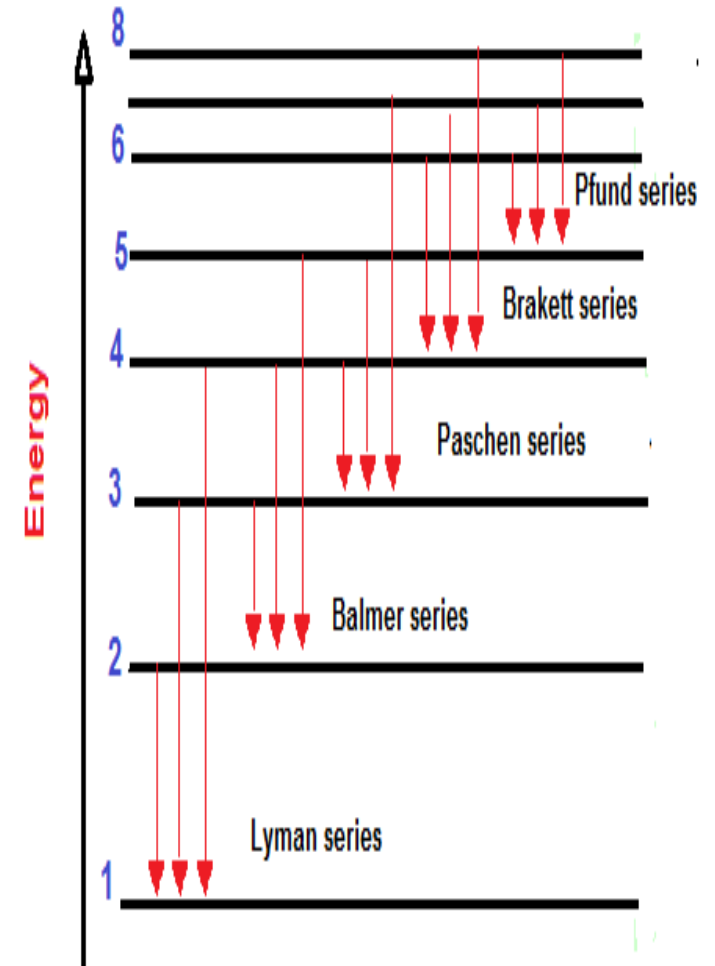
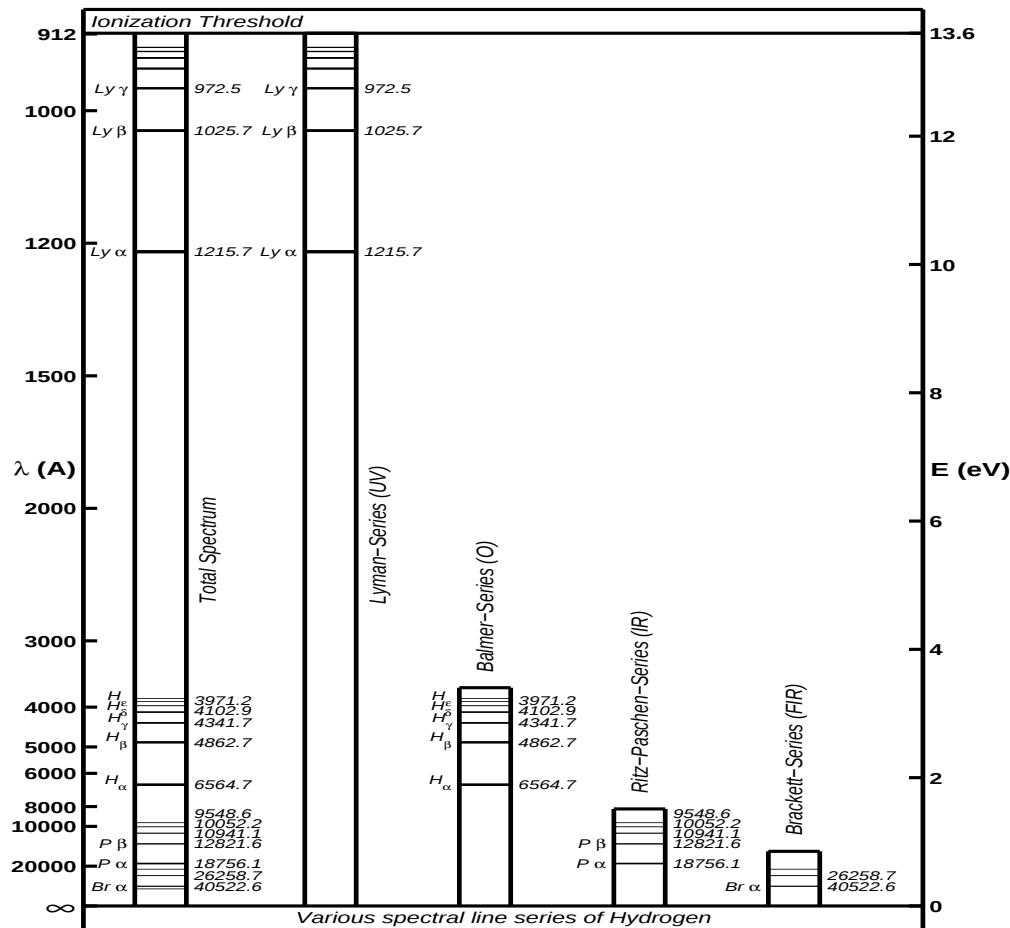
$$\mathcal{R}_H \left[\frac{1}{2^2} - \frac{1}{n'^2} \right], \quad n' = 3, 4, 5, \dots \quad \text{Balmer (Ba)}$$

$$\mathcal{R}_H \left[\frac{1}{3^2} - \frac{1}{n'^2} \right], \quad n' = 4, 5, 6, \dots \quad \text{Paschen (Pa)}$$

$$\mathcal{R}_H \left[\frac{1}{4^2} - \frac{1}{n'^2} \right], \quad n' = 5, 6, 7, \dots \quad \text{Brackett (Br)}$$

$$\mathcal{R}_H \left[\frac{1}{5^2} - \frac{1}{n'^2} \right], \quad n' = 6, 7, 8, \dots \quad \text{Pfund (Pf)}$$

HYDROGEN SPECTRUM & EI



- Lyman series: 1215 – 912 Å (Far ultra-violet FUV), Balmer series: 6564 – 3646 Å (Optical O & Near UV), Paschen series: 18751 – 8204 Å (Near IR NIR), Brackett series: Far IR (FIR)
- For each series, Δn sequence is defined with α , β , γ , δ , etc.,
Ex: Lyman series: Ly α (1215.67 Å), Ly β (1025.72 Å), Ly γ (972.537 Å..., Ly $_{\infty}$ (911.76 Å)
- Ly α - (1s-2p) is "the resonance line"

ASTROPHYSICAL SPECTROSCOPY: IDENTIFICATION OF LINES

- We study atoms and ions experimentally and theoretically and determine the atomic energies and transition lines with their energies, mainly in wavelengths, and make them publicly available by publications and data tables, such as, the National Institute of Standards and Technology (NIST) in the USA
- Each atomic system has its own set of energies and transitions. But lines can form at the same wavelength by two different atomic species which we call blend. In such case we need some additional information
- Through ground- or space-based telescopes, we take the spectrum of an astronomical object and clean out the noise introduced by the observing equipment - data reduction
- We match the observed lines with those pre-existing lines and identify the element that produced those lines.
- Existence of an observed line depends on the atomic processes of photo-excitation, electron-ion excitation, photoionization, electron-ion recombination which can occur in empty space or in a plasma environment. In pure atomic physics, theoretical or experimental, lines are studied independent of the environment. These can go in model where plasma effects on the lines are incorporated.
- Observation of a sharp line typically indicates thin and cool plasma not affecting the atomic system

ASTROPHYSICAL SPECTROSCOPY: PLASMA EFFECTS ON LINES

- The intensity of the observed line depends on
 - population of transitional levels which can be caused by the atomic processes, and
 - environmental factors such as density and temperature of the plasmaTo study these, we need plasma modeling using the pure atomic data
- The width of a line of an atomic system can be broadened mainly by three factors in the dense and high temperature plasma:
 - Collisional broadening when low level excitation energy is added to the line by electron impact
 - Doppler broadening when the atomic species moving fast in the plasma
 - Stark broadening when the surrounding close-by ions affecting the atomic system by their electromagnetic field which can reduce the ionization energy and lower the levels.
- Line broadening means when spectral lines are broaden and continuum broadening means when the spectral background shows the effect such as due to dissolving photoionization resonances or weak bound-bound transition
- When single lines are observed, they can be simulated by broadening theoretical spectra with a gaussian profile function. The function does not depend on the temperature and density of the plasmas