

Interstellar Medium (ISM)

Week 2

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- Heating & Cooling -

- Heating processes
 - The primary heating mechanisms of the ISM involve providing free electrons with high energies. Through collisions, the fast free electrons share their kinetic energy with other particles, and through further collisions, the distribution of velocities approaches a Maxwellian distribution.
 - ***Source of free electrons:*** The fast electrons may have been ejected from atoms by cosmic rays, from dust grains by photons or from atoms by photons or they may have been accelerated by shocks.
 - ◆ **Ionization by cosmic rays**
 - ◆ **Photoionization of dust grains by starlight UV.**
 - ◆ **Photoionization of atoms (H, He, C, Mg, Si, Fe, etc) by X-rays or starlight UV.**
 - **Other heating sources:**
 - ◆ **Heating by shock waves and other MHD phenomena.**
- Cooling processes
 - Collisional excited lines ([C II], [O I], Ly α , etc)
 - Thermal bremsstrahlung

(2) Photoelectric Heating by Dust

- UV and X-ray photons can knock electrons free from dust grains. The ejected electrons carry kinetic energy, which can be effective at heating the surrounding gas.
- ***Photoelectrons emitted by dust grains dominate the heating of the diffuse neutral ISM (CNM and WNM) in the Milky Way.***
- The work function, analogous to the ionization energy of an atom, for graphite is 4.50 ± 0.05 eV. Therefore, UV photons with $h\nu \gtrsim 5$ eV can kick out photoelectrons from dust grains. The photoelectric heating by dust is dominated by photons with $h\nu \gtrsim 8$ eV.

$$G_{\text{pe}} \approx 2 \times 10^{-26} \frac{n_{\text{ph}}(8 - 13.6 \text{ eV})}{4.3 \times 10^{-3} \text{ cm}^{-3}} \frac{\langle \sigma_{\text{abs}} \rangle}{10^{-21} \text{ cm}^2} \frac{\langle Y \rangle}{0.1} \frac{\langle E_{\text{pe}} \rangle - \langle E_c \rangle}{1 \text{ eV}} \text{ erg s}^{-1}$$

The gain is independent of temperature.

Here,

$n_{\text{ph}}(8 - 13.6 \text{ eV})$ = number density of $8 < h\nu < 13.6$ eV photons

$\langle \sigma_{\text{abs}} \rangle$ = total dust photo absorption cross section per H nucleon, averaged over the photon spectrum.

$\langle Y \rangle$ = photoelectric yield averaged over the spectrum of 8 to 13.6 eV photons absorbed by the interstellar grain mixture.

$\langle E_{\text{pe}} \rangle$ = mean kinetic energy of escaping photoelectrons.

$\langle E_c \rangle$ = mean kinetic energy of electrons captured from the plasma by grains.

- ***Photoelectric heating from dust may be an order of magnitude larger than the cosmic ray heating rate.***

- Cooling -

- [C II] 158μm (collisionally excited line emission)
 - The electronic ground state of C II is split into two fine levels, separated by an energy $E_{ul} = 7.86 \times 10^{-3}$ eV, which corresponds to $\lambda = 158 \mu\text{m}$ and $T = E_{ul}/k = 91.2 \text{ K}$.
 - The upper level is populated by collisions with hydrogen atoms and free electrons.
 - If C II is excited by collisions with free electrons, the cooling function is given by, for a C abundance $n_C/n_H = 2.7 \times 10^{-4}$,

$$\frac{\Lambda_{[\text{CII}]}^e}{10^{-27} \text{ erg cm}^3 \text{ s}^{-1}} \approx 3.1 \left(\frac{x}{10^{-3}} \right) \left(\frac{T}{100 \text{ K}} \right)^{-1/2} \exp \left(-\frac{91.2 \text{ K}}{T} \right)$$

Here, $x = n_e/n$ is the ionization fraction.

- If the C II is excited by collisions with hydrogen atoms, the cooling function is

$$\frac{\Lambda_{[\text{CII}]}^H}{10^{-27} \text{ erg cm}^3 \text{ s}^{-1}} \approx 5.2 \left(\frac{T}{100 \text{ K}} \right)^{0.13} \exp \left(-\frac{91.2 \text{ K}}{T} \right)$$

- In the CNM, both contribute significantly to the excitation of C II.

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- [O I] 63.2 μm (collisionally excited emission line)
 - The electronic ground state of O I has a fine splitting of $E_{u\ell}/k = 228 \text{ K}$.
 - The upper level is populated primarily by collisions with hydrogen atoms.
 - The resulting cooling function due to the emission of 63.2 μm is, for an abundance of $n_{\text{O}}/n_{\text{H}} = 6.0 \times 10^{-4}$,

$$\frac{\Lambda_{[\text{OI}]}^{\text{H}}}{10^{-27} \text{ erg cm}^3 \text{ s}^{-1}} \approx 4.1 \left(\frac{T}{100 \text{ K}} \right)^{0.42} \exp \left(-\frac{228 \text{ K}}{T} \right)$$

At $n_{\text{O}}/n_{\text{C}} = 2.2$, cooling by O I doesn't surpass cooling by C II until T reaches $\sim 800 \text{ K}$.

- Note:
 - [C II] and [O I] are the dominant form of cooling in molecular clouds and the CNM.
 - Molecular clouds can also cool by emission from the vibrational and rotational transitions of molecules.
 - The critical densities for [C II] and [O I] are $\sim 4 \times 10^3 \text{ cm}^{-3}$ and $\sim 10^5 \text{ cm}^{-3}$, respectively, implying that collisional deexcitation of these levels is unimportant in the diffuse ISM of the Milky Way.

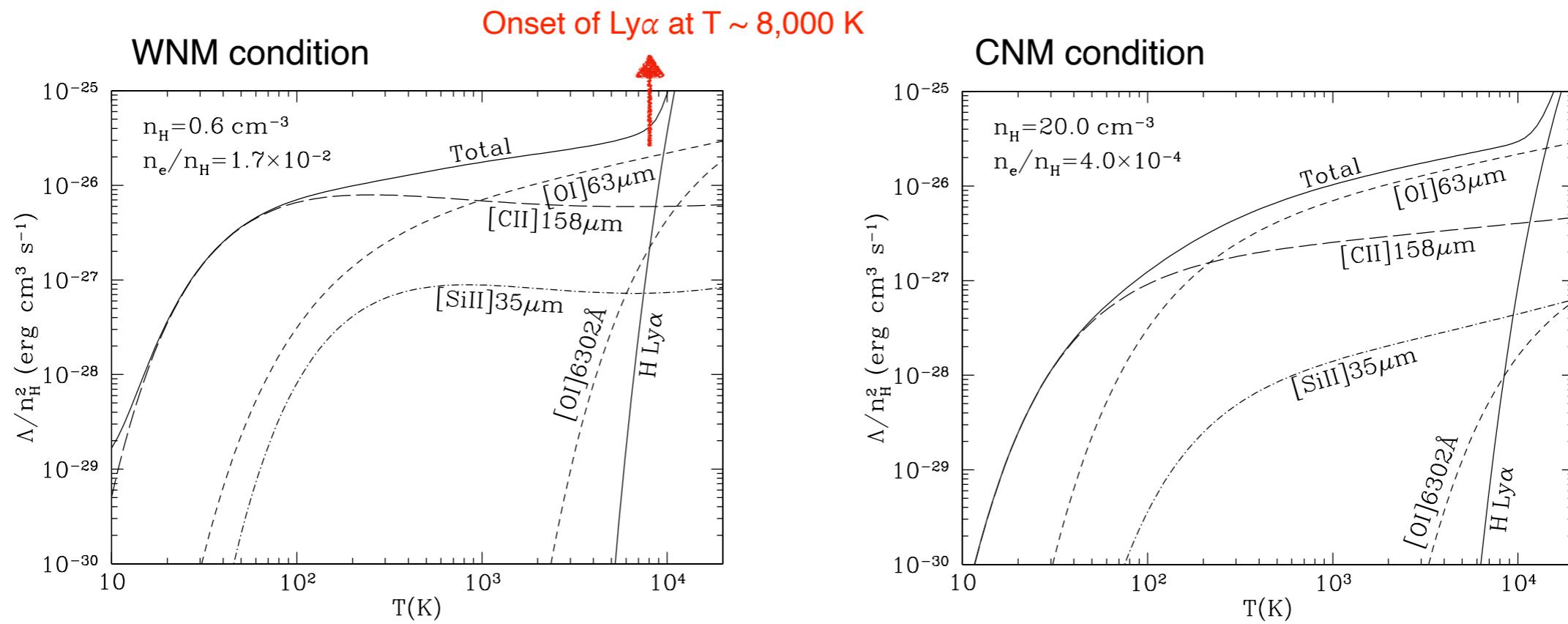
- Collisionally excited Ly α 1216Å

- The first excited level of atomic hydrogen is $E_{21} = 10.20 \text{ eV}$ above the ground state.
- Although the first excited level will not be highly populated by collisions until the temperature reaches $T \sim E_{21}/k = 118,000 \text{ K}$. However, there are ~ 1700 H atoms for every O atom. In addition, Ly α photon carries away ~ 520 times as much energy as an O I photon. Thus the cooling by Ly α can compete with cooling by IR fine-structure lines at temperature as low as $T \approx 10^4 \text{ K}$.
- The cooling function for H excited by collisions with free electrons is

$$\frac{\Lambda_{[\text{Ly}\alpha]}^e}{10^{-27} \text{ erg cm}^3 \text{ s}^{-1}} \approx 6 \times 10^5 \left(\frac{x}{10^{-3}} \right) \left(\frac{T}{100 \text{ K}} \right)^{-0.5} \exp \left(-\frac{118,000 \text{ K}}{T} \right)$$

- When $T > 20,000 \text{ K}$,
 - atomic hydrogen can be collisionally ionized, followed by radiative recombination to a high energy level, and followed by a cascade down to the ground state.
 - The recombination lines from hydrogen are an important cooling mechanism in the WNM and WIM.
 - These phases are also cooled by line emission from more highly ionized atoms such as O III, C IV, and O VI.

- Free-free emission (Thermal Bremsstrahlung)
 - In the HIM at $T > 10^6$ K, the “braking radiation” emitted by electrons when they are accelerated by other charged particles can be a significant cooling mechanism.
 - The cooling function is $\Lambda \propto T^{1/2}$.
- Cooling Function

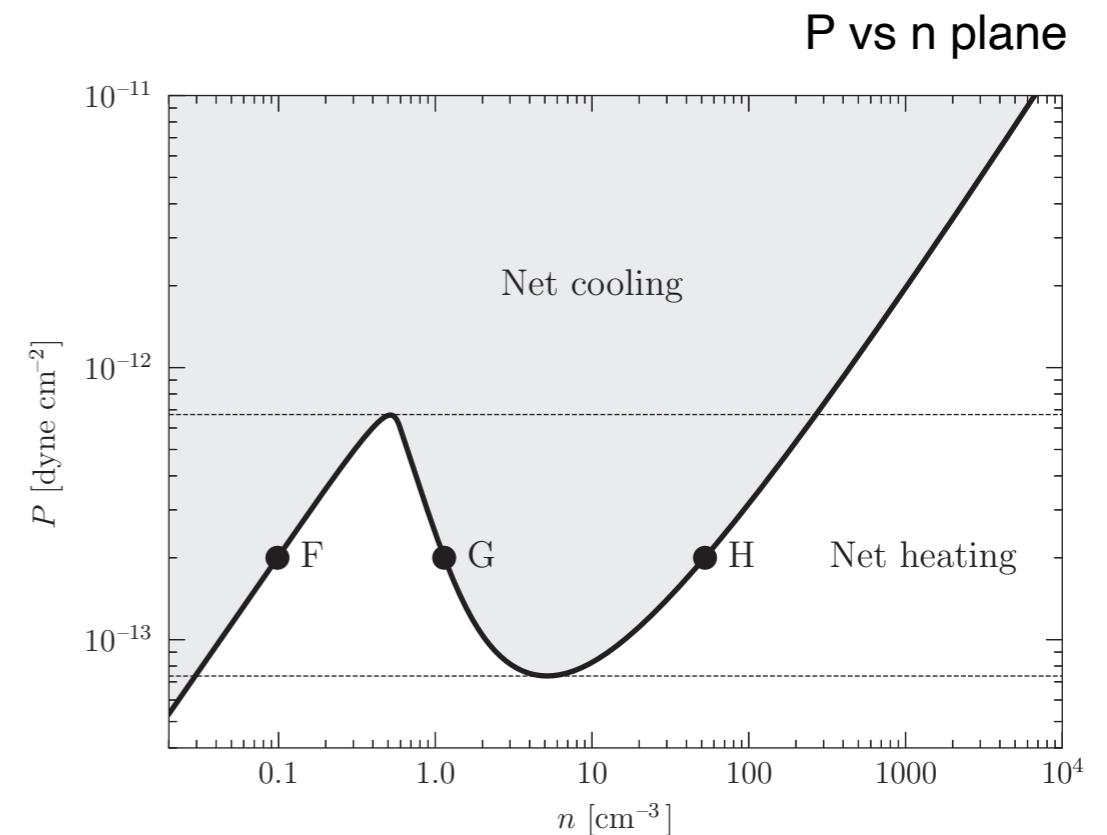
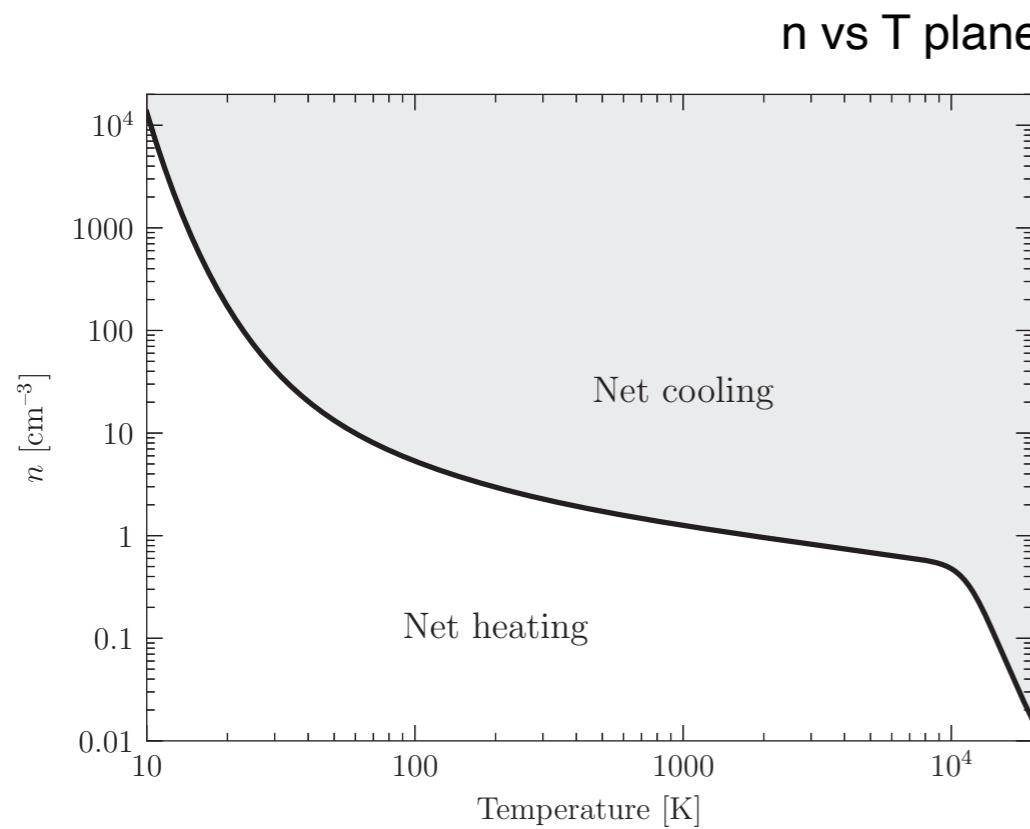


- For $10 < T < 10^4$ K, [C II] 158 μm line is a major coolant. The [O I] 63 μm line is important for $T > 100$ K. Lyα cooling dominates only at $T > 10^4$ K.

Stable & Unstable Equilibrium

- A thermal equilibrium must have heating and cooling balanced: $g = \ell$.
 - We assume ***photoelectric heating by dust*** and ***cooling by [C II], [O I], and Ly α*** . Then, the equilibrium density is obtained by

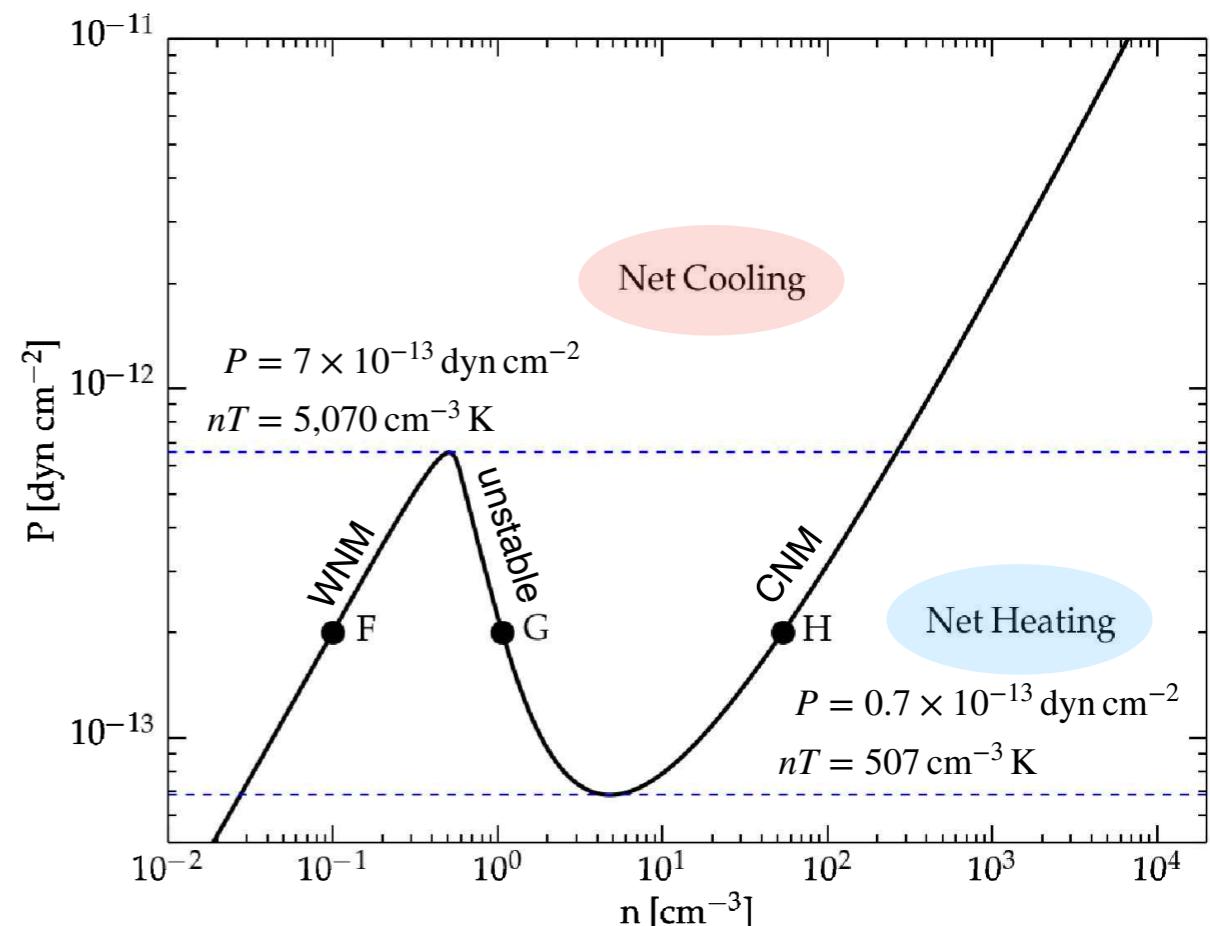
$$n_{\text{eq}} G = n_{\text{eq}}^2 \Lambda \quad \rightarrow \quad n_{\text{eq}}(T) = \frac{G}{\Lambda(T)} \quad \text{Note that } G \text{ is a (nearly) constant.}$$



- If every point along the above equilibrium line represented a stable equilibrium, then there could be a continuous distribution of temperatures, and thus of number densities.
- However, it's not the case. Not every equilibrium point is a stable equilibrium.
- The presence of distinct phases in the ISM results from the distinction between stable and unstable equilibrium.

- Pressure Equilibrium

- Let's assume that the interstellar gas is in pressure equilibrium.
- For pressures in the range $0.7 \times 10^{-13} \text{ dyn cm}^{-2} < P < 7 \times 10^{-13} \text{ dyn cm}^{-2}$, bounded by the dashed lines, **there are three possible values of n_{eq} at a fixed pressure**.
- Consider what happens at a point, for instance F, if you slightly change the temperature while keeping the pressure fixed.
 - If T increases, n must decrease, and you must move left from point F. This moves you into the net cooling portion, and T consequently decreases.
 - If T decrease, n must increase, and this moves you rightward into the net heating portion, and T consequently increases.
 - Thus, a negative feedback restores the original temperature.
- A similar negative feedback maintains temperature stability at point H.
- However, now consider what happens at G.
 - If T increases, n must decrease, and you must move left from point G. This moves you into the net heating portion, and T increases further, until you reach F.
 - If T decrease, n must increase, and this moves you rightward into the net cooling portion, and T decrease further, until you reach H.
 - Thus, a positive feedback makes the point unstable.
- **Consequently, we have two stable equilibrium points (F and H). F = WNM, H = CNM**

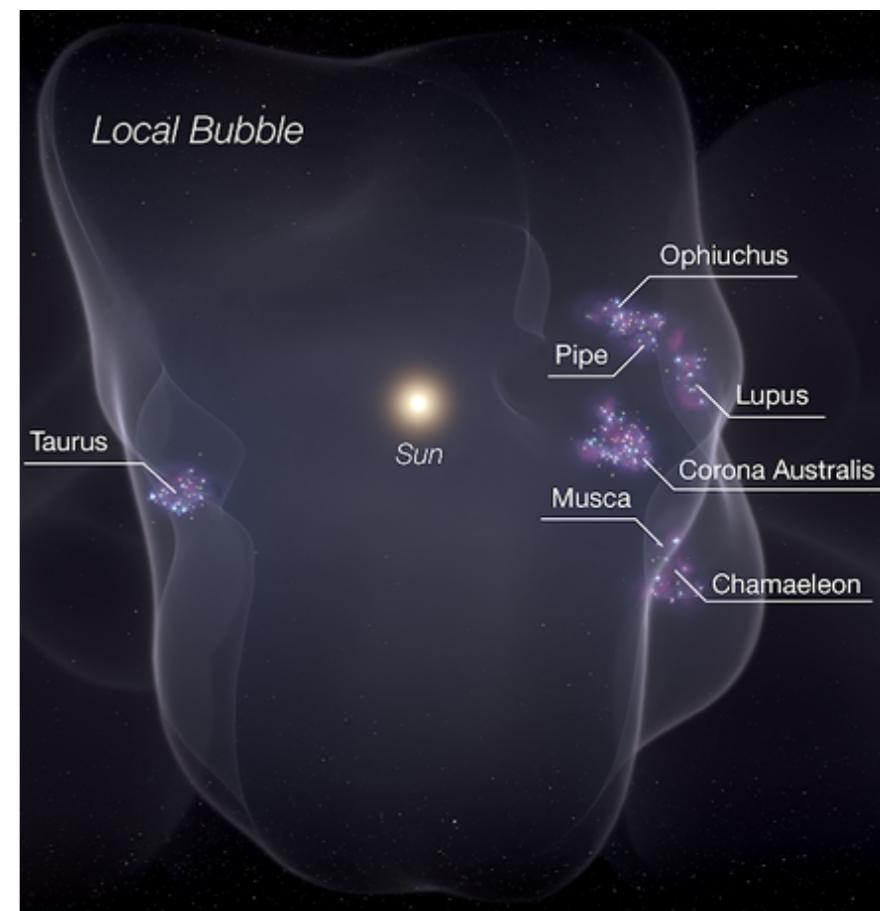


- History: Two-Phase Model & Three-Phase Model

- As a result of their analysis, ***Field, Goldsmith, and Habing (1969)*** created a two-phase model of the ISM, consisting of Cold Neutral Clouds, with $n \sim 10 \text{ cm}^{-3}$ and $T \sim 100 \text{ K}$, embedded within a Warm Intercloud Medium, with $n \sim 0.1 \text{ cm}^{-3}$ and $T \sim 10,000 \text{ K}$.
 - ◆ They were unaware of the role played by dust in heating the ISM, assumed that ***collisional ionization by cosmic rays provided the bulk of the heating.***
 - ◆ FGH (1969) advocated a two-phase model. However, they also speculated “an existence of a third stable phase at $T > 10^6 \text{ K}$, with bremsstrahlung the chief cooling process.”
- In the 1970s, detection of a diffuse soft X-ray background and of emission lines such as O VI 1032, 1038Å hinted at the existence of interstellar gas with $T \sim 10^6 \text{ K}$. In fact, the Sun resides in a “***Local Bubble***” of hot gas, with $T \sim 10^6 \text{ K}$ and $n \sim 0.004 \text{ cm}^{-3}$.
- Cox & Smith (1974) suggested that supernova remnants could produce a bubbly hot phase, and that the bubbles blown by supernovae would have a porosity factor (volume fraction of the ISM occupied by hot bubbles):

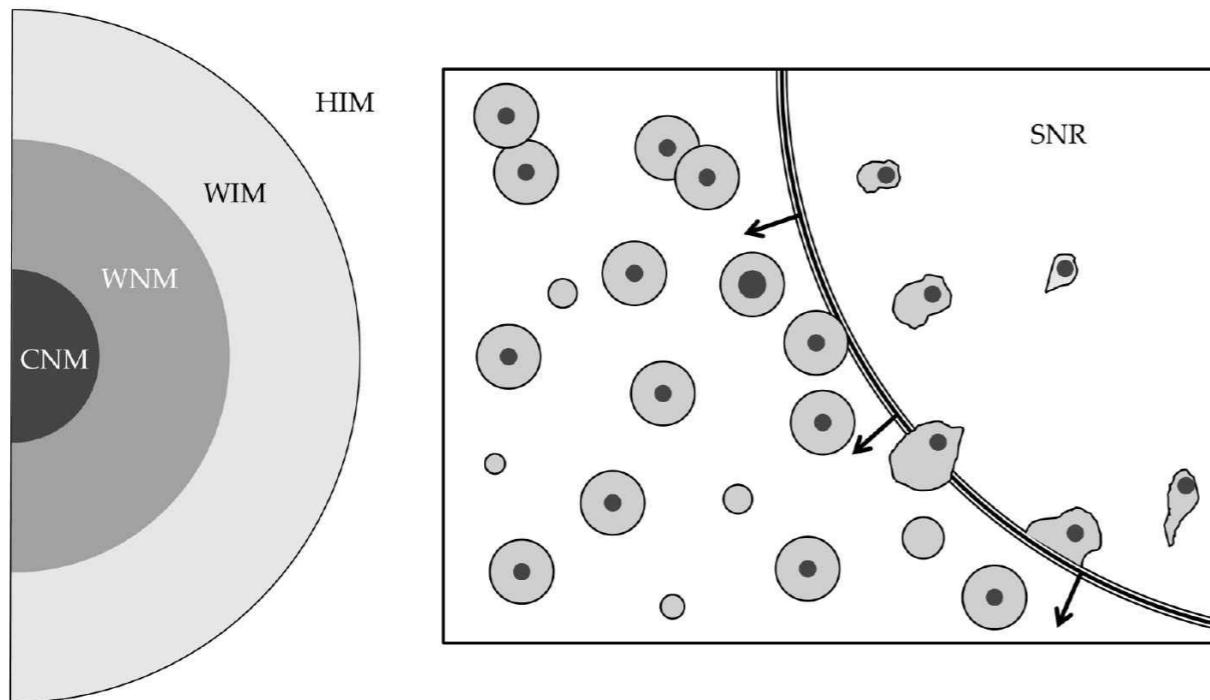
porosity factor: $q > 0.1 \left(\frac{r_{\text{SN}}}{10^{-13} \text{ pc}^{-3} \text{ yr}^{-1}} \right)$ r_{SN} is the supernova rate per unit volume.

 - If $0.1 < q < 0.5$, the expanding supernova remnants can join to form supersized bubbles and elongated tunnels of hot gas.
 - A superbubble or supershell is a cavity which is $\sim 100 \text{ pc}$ across and is populated with hot (10^6 K) gas atoms, less dense than the surrounding ISM, blown against that medium and carved out by multiple supernovae and stellar winds.



- History: McKee & Ostriker's Three-Phase Model

- McKee & Ostriker (1977)
 - They made a more elaborate argument for three phases within the ISM.
 - **Cold Neutral Medium**, with $T \sim 80$ K, $n \sim 40 \text{ cm}^{-3}$, and a low fractional ionization $x = n_e/n \sim 0.001$.
 - **Warm Medium**, containing both ionized and neutral components, $T \sim 8000$ K and $n \sim 0.3 \text{ cm}^{-3}$, the ionization fraction ranging from $x \sim 0.15$ in the neutral component (WNM) to $x \sim 0.7$ in the ionized component (WIM).
 - **Hot Ionized Medium**, consisting of the overlapping supernova bubbles, with $T \sim 10^6$ K and $n \sim 0.002 \text{ cm}^{-3}$, and $x \sim 1$ (nearly complete ionization).



The left panel shows a typical cold neutral cloud, surrounded by the warm medium (WNM and WIM).

The right panel shows an expanding supernova blastwave overtaking a population of cold clouds.

- However, in many ways, the ISM is a dynamic, turbulent, dusty, magnetized place.
- The five-phase model is largely empirical (not relying on assumptions about thermal pressure equilibrium).

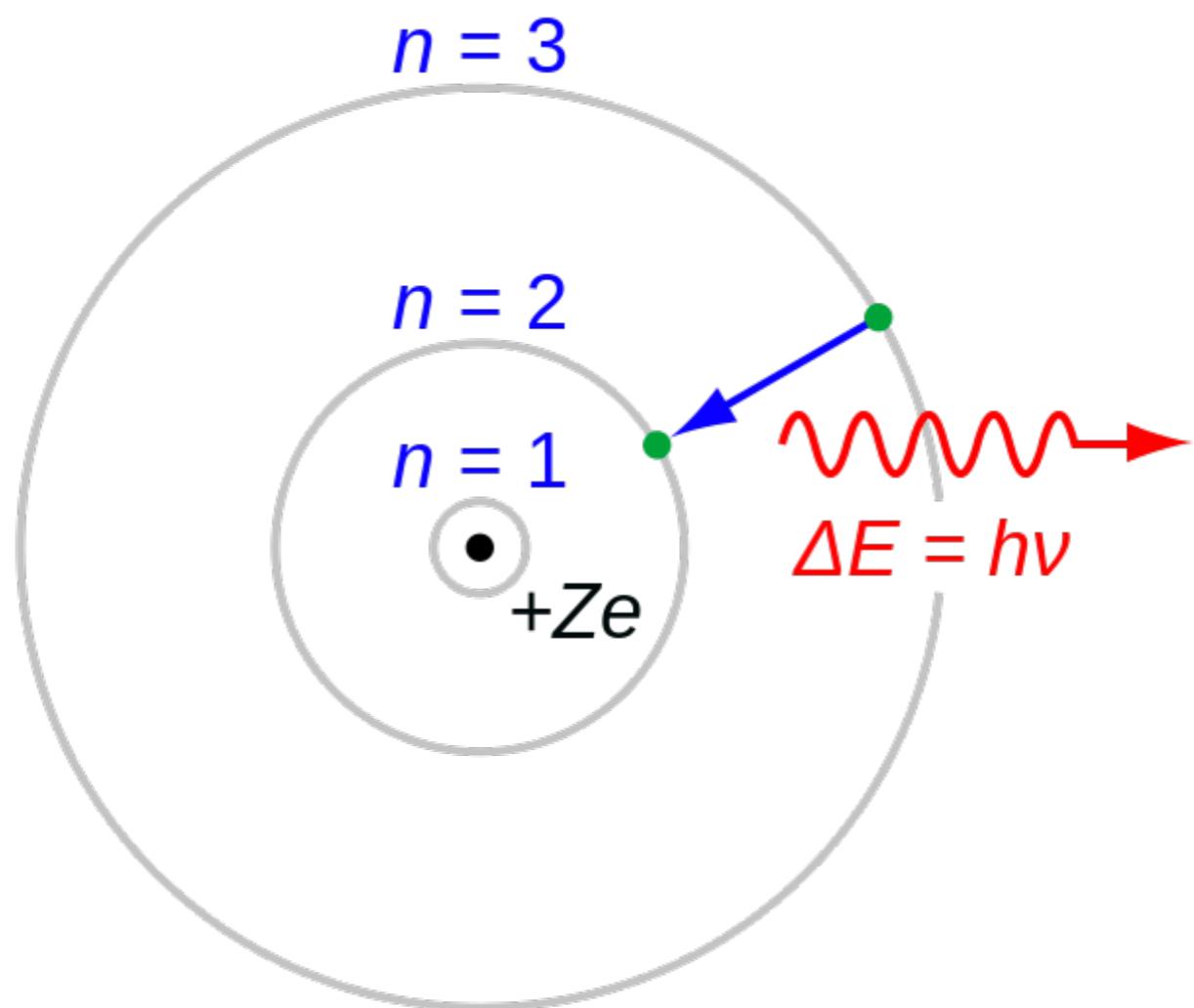
Atomic Structure, Spectroscopy

References

- Books for atomic/molecular structure and spectroscopy
 - Astronomical Spectroscopy [Jonathan Tennyson]
 - Physics of the Interstellar and Intergalactic Medium [Bruce T. Draine]
⇒ see <https://www.astro.princeton.edu/~draine/> for errata
 - Astrophysics of the Diffuse Universe [Michael A. Dopita & Ralph S. Sutherland]
⇒ many typos
 - Physics and Chemistry of the Interstellar Medium [Sun Kwok]
 - Atomic Spectroscopy and Radiative Processes [Egidio Landi Degl'Innocenti]

Quantum Mechanics: Bohr model

- In atomic physics, the Bohr model, consists of a small, dense nucleus surrounded by orbiting electrons.
 - The negatively charged electron confined to an atomic shell encircles a small, positively charged atomic nucleus and where an electron jumps between orbits, is accompanied by an emitted or absorbed amount of electromagnetic energy.



Quantum Mechanics: Hydrogen Atom

- Each bound state of the hydrogen atom is characterized by a set of four quantum numbers (n, l, m, m_s)

- $n = 1, 2, 3, \dots$: principal quantum number
- $l = 0, 1, 2, \dots, n - 1$: orbital angular momentum quantum number
 - By convention, the values of l are usually designated by letters.

0	1	2	3	4	5	6	7	8	...
s	p	d	f	g	h	i	k	l	...

- $m = -l, -l + 1, \dots, 0, \dots, l - 1, l$: magnetic quantum number.
 - It determines the behavior of the energy levels in the presence of a magnetic field.
 - This is the projection of the electron orbital angular momentum along the z -axis of the system.

- Spin

- The electron possesses an intrinsic angular momentum with the magnitude of $|s| = \frac{1}{2}$.
- There are two states, $m_s = \pm \frac{1}{2}$, for the spin.

- Degeneracy for a given n : $2 \times \sum_{l=0}^{n-1} (2l + 1) = 2n^2$

Schrödinger Equation

- A good starting point for a quantum mechanical understanding of spectral lines is the hydrogen atom, which is the simplest of all atoms, consisting of one proton and one electron.
- Since the H atom consists of only a proton and an electron, the Coulomb field experienced by the electron is spherically symmetric. The time-dependent Schrödinger equation for a system with **Hamiltonian H**:

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$$

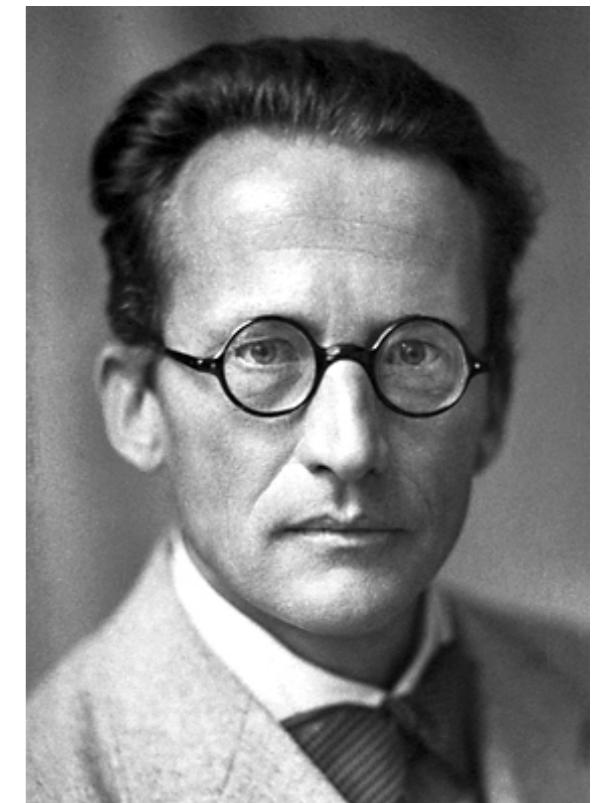
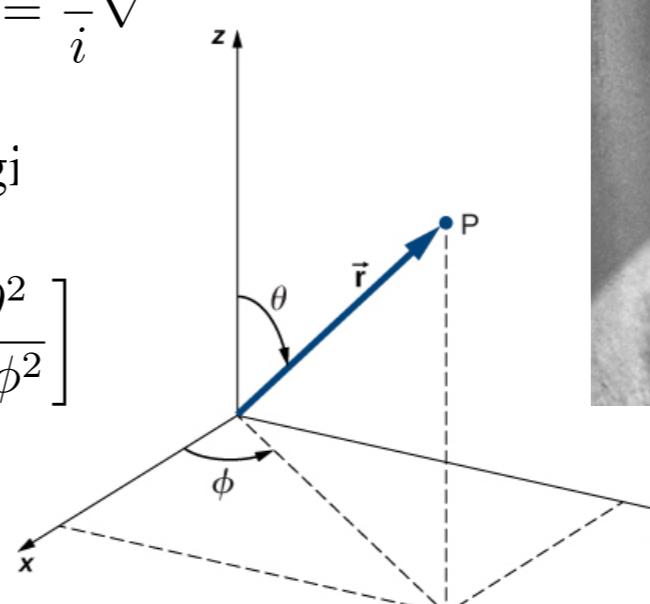
Often we are interested in the stationary solutions found by separating the time and space parts of the wave function, which is possible *if H is independent of time*:

- The time-independent Schrödinger equation is obtained as follows:

$$\begin{aligned}\Psi(\mathbf{r}, t) &= \psi(\mathbf{r})e^{iEt/\hbar} \longrightarrow H\psi(\mathbf{r}) = E\psi(\mathbf{r}) \\ H &= \frac{p^2}{2m} + V(r) = -\frac{\hbar^2}{2m}\nabla^2 + V(r)\end{aligned}$$

momentum operator:

$$\mathbf{p} = \frac{\hbar}{i}\nabla$$



Erwin Schrödinger

$$\begin{aligned}\nabla^2 &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \\ &= \mathcal{R} + \frac{1}{r^2} \mathcal{L}^2\end{aligned}$$

Here, in the spherical coordinates, the Laplace operator is given by

Solution for the Hydrogen atom

- momentum operator $\mathbf{p} = \frac{\hbar}{i}\nabla$
- Hamiltonian operator $H = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\nabla^2 + V$
- Expectation value of an operator

$$\langle F \rangle = \int \psi^* F \psi d^3x \quad \rightarrow \quad \langle F \rangle = \langle \psi | F | \psi \rangle$$

- Wavefunction for a hydrogen-like atom:

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)Y_{lm}(\theta, \phi)$$

radial function:

$$R_{nl}(r) = - \left[\left(\frac{2Z}{na_0} \right)^3 \frac{(n-l-1)!}{2n\{(n+l)!\}^3} \right]^{1/2} e^{-\rho/2} \rho^l L_{n+l}^{2l+1}(\rho)$$

$$\rho = \frac{2Z}{na_0}r, \quad a_0 \equiv \frac{\hbar^2}{m_e c^2} = 0.529\text{\AA} \text{ (Bohr radius)},$$

L_{n+l}^{2l+1} = associated Laguerre polynomial

spherical harmonics

$$Y_{lm}(\theta, \phi) = (-1)^{(m+|m|)/2} \left[\frac{(l-|m|)!}{(l+|m|)!} \frac{2l+1}{4\pi} \right]^{1/2} P_l^{|m|}(\cos \theta) e^{im\phi}$$

$P_l^{|m|}$ = associated Legendre function

- $n = 1, 2, 3, \dots$: **principal quantum number**
- $l = 0, 1, 2, \dots, n-1$: **orbital angular momentum quantum number**
- $m = -l, -l+1, \dots, 0, \dots, l-1, l$: **magnetic quantum number**

bra-ket notation (Dirac notation)
ket vector : $|\psi\rangle$
bra vector : $\langle\phi| = |\psi\rangle^\dagger$
(\dagger : conjugate transpose)

- Wavefunctions for a hydrogen-like atom

Atomic Physics [Foot]

$$R_{1,0} = \left(\frac{Z}{a_0}\right)^{3/2} 2 e^{-\rho}$$

$$R_{2,0} = \left(\frac{Z}{2a_0}\right)^{3/2} 2(1-\rho) e^{-\rho}$$

$$R_{2,1} = \left(\frac{Z}{2a_0}\right)^{3/2} \frac{2}{\sqrt{3}} \rho e^{-\rho}$$

$$R_{3,0} = \left(\frac{Z}{3a_0}\right)^{3/2} 2 \left(1 - 2\rho + \frac{2}{3}\rho^2\right) e^{-\rho}$$

$$R_{3,1} = \left(\frac{Z}{3a_0}\right)^{3/2} \frac{4\sqrt{2}}{3} \rho \left(1 - \frac{1}{2}\rho\right) e^{-\rho}$$

$$R_{3,2} = \left(\frac{Z}{3a_0}\right)^{3/2} \frac{2\sqrt{2}}{3\sqrt{5}} \rho^2 e^{-\rho}$$

Normalisation: $\int_0^\infty R_{n,l}^2 r^2 dr = 1$

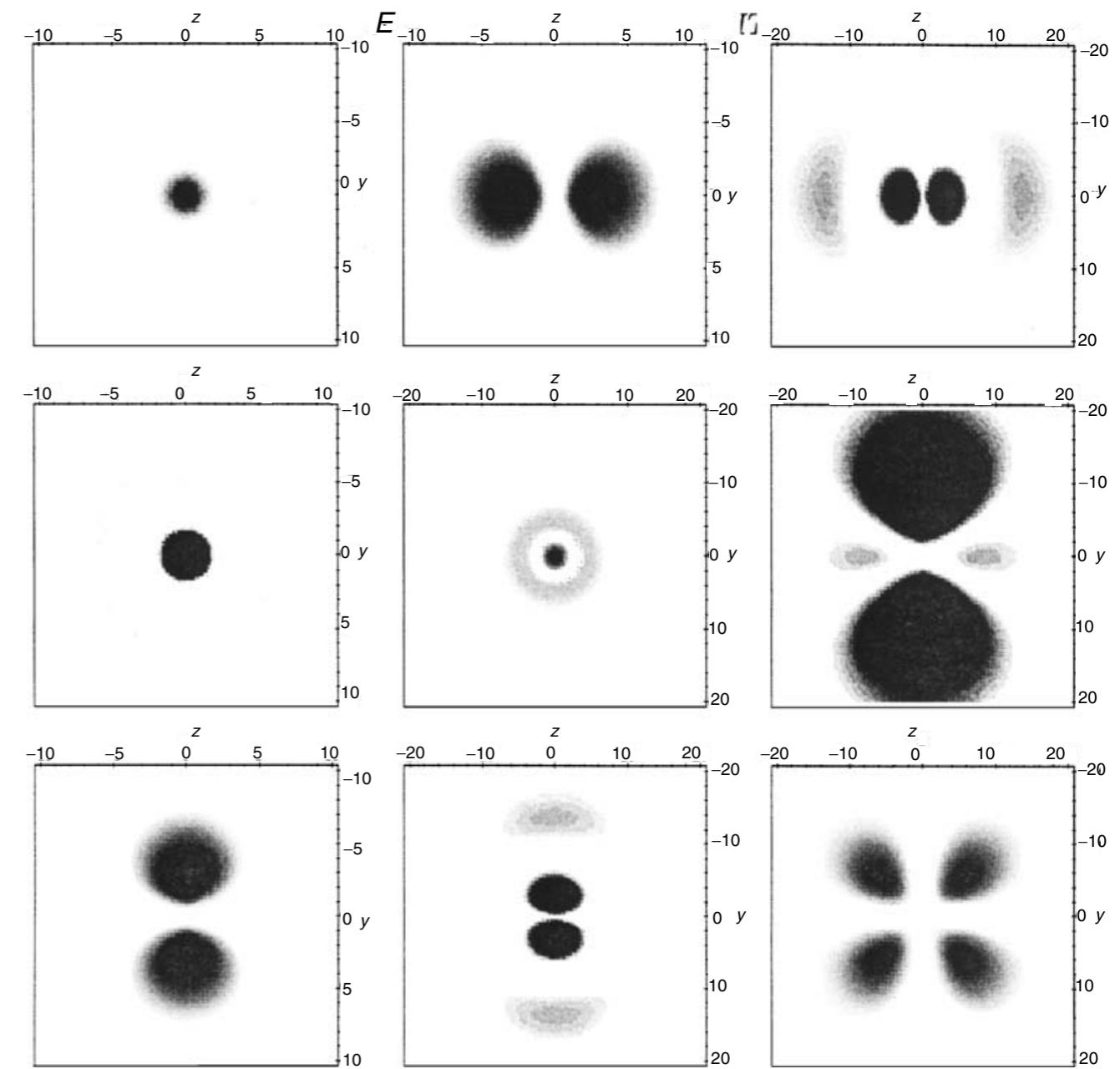
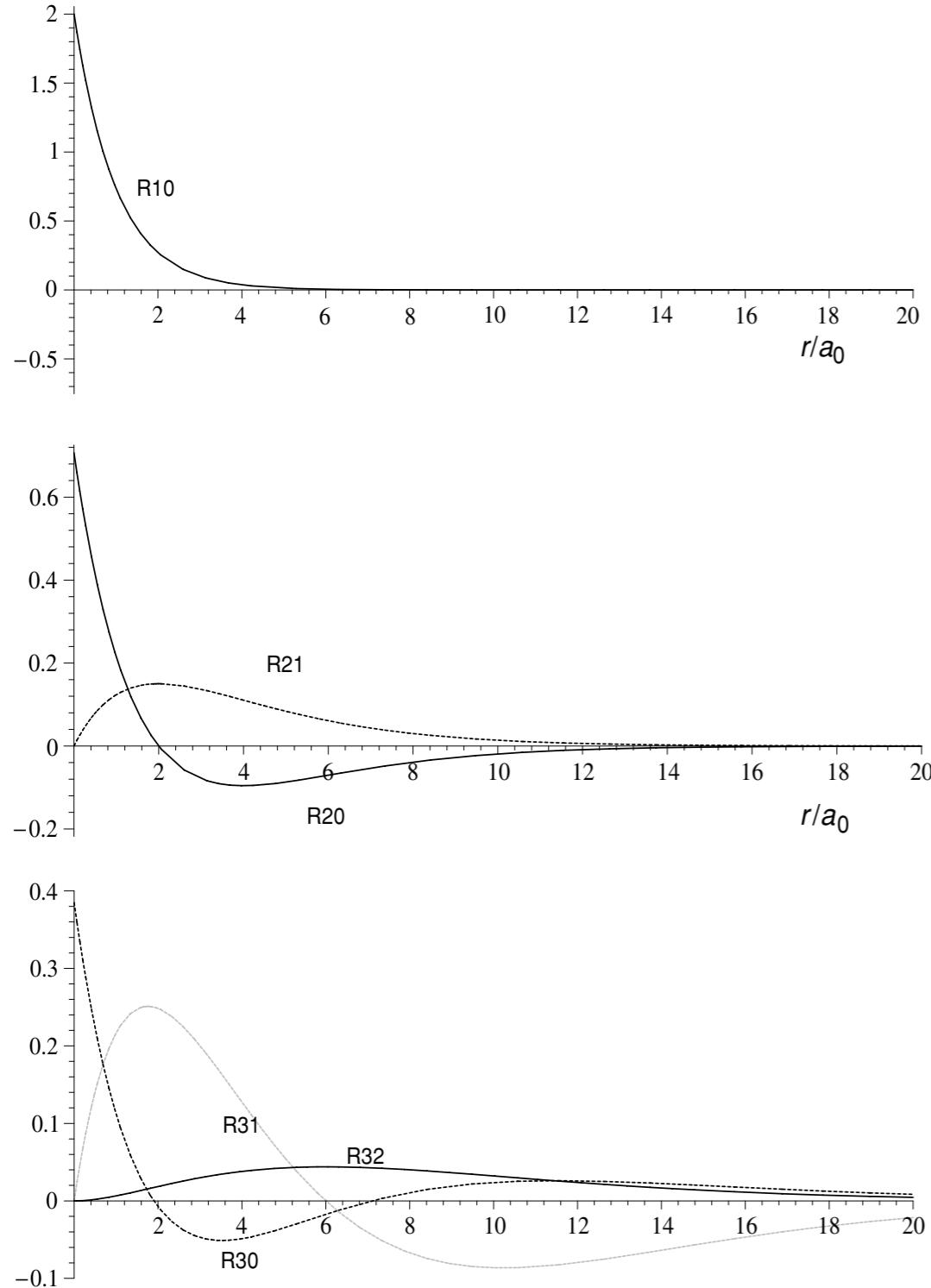
Here, $\rho \equiv \frac{Z}{na_0}r$

- Probability: $|\psi(r, \theta, \phi)|^2 d^3x = R_{nl}^2(r) |Y_{lm}(\theta, \phi)|^2 r^2 \sin \theta dr d\theta d\phi$

- Properties of the spherical harmonics: $\int_0^\pi \int_0^{2\pi} |Y_{lm}(\theta, \phi)|^2 \sin \theta d\theta d\phi = 1$

$$\sum_{m=-l}^l |Y_{lm}(\theta, \phi)|^2 = \frac{2l+1}{4\pi}$$

This implies that **closed shells are spherically symmetric and have very little interaction with external electrons.**



Probability distributions (per unit volume). A slice through the $\phi = 0$ plane. The darker the shading the greater the probability density.

[Left] 1s, 2s, 2p0 from top to bottom
 [Center] 2p1, 3s, 3p0
 [Right] 3p1, 3d0, 3d1

[Angular Momentum]

- The orbital angular momentum operator $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ has the following eigenvalue. The spherical harmonics are eigenfunctions of the orbital angular momentum operator

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = \frac{\hbar}{i} \mathbf{r} \times \nabla$$

$$\mathbf{L}^2 Y_{lm} = l(l+1)\hbar^2 Y_{lm}, \quad L_z Y_{lm} = m\hbar Y_{lm}$$

Here, the ℓ can have values $\ell = 0, 1, \dots, n - 1$.

The magnitude of the angular momenta are

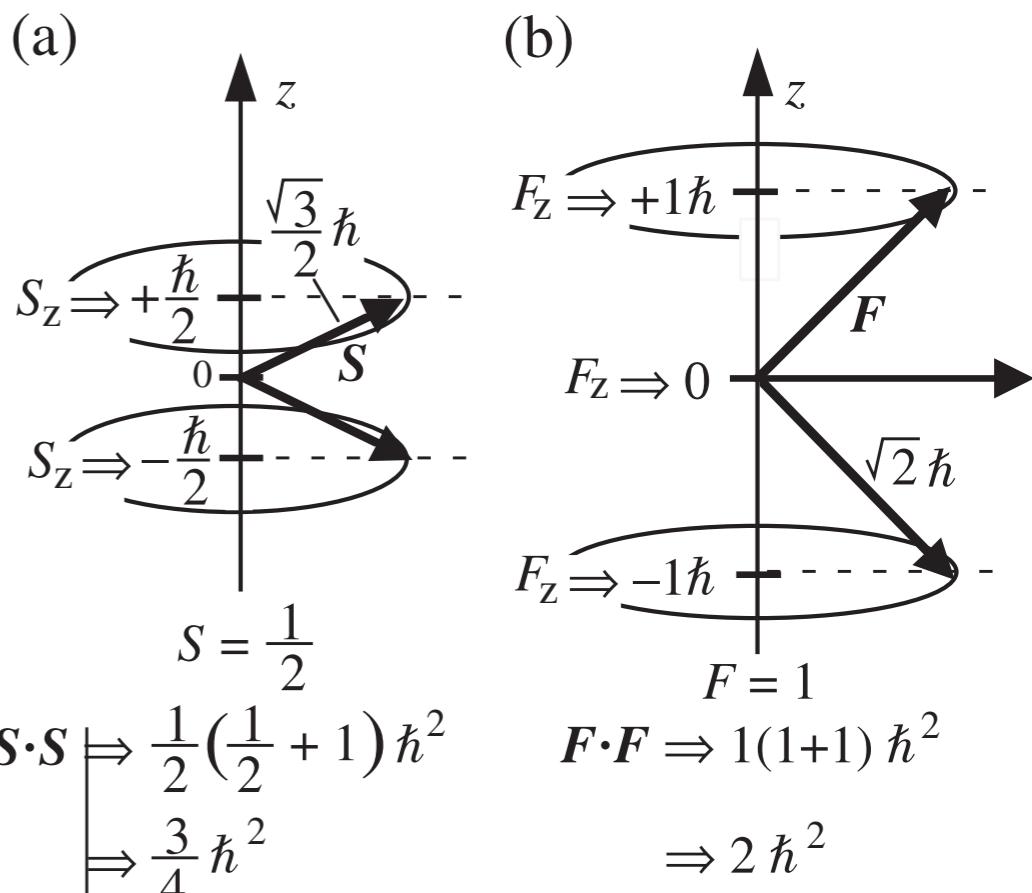
$$|\mathbf{L}| = \sqrt{\ell(\ell+1)}\hbar \quad \text{where } \ell = 0, 1, \dots, n - 1$$

The z -component have the following values.

$$L_z = m\hbar \quad \text{where } m = -\ell, -\ell+1, \dots, \ell-1, \ell$$

- Electron has a spin of $s = \frac{1}{2}$ and it has two z -components:

$$s = \frac{1}{2}\hbar \rightarrow m_s = -\frac{1}{2}\hbar, \frac{1}{2}\hbar$$



Many electron systems : Schrödinger Equation

- The time-independent Schrödinger equation for an atom with N electrons and nuclear charge (atomic number) Z .

$$\left[\sum_{i=1}^N \left(-\frac{\hbar^2}{2m} \nabla_i^2 - \frac{Ze^2}{r_i} \right) + \sum_{i=1}^{N-1} \sum_{j=1}^N \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \right] \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = E \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$$

where \mathbf{r}_i is the coordinate of the i th electron, with its origin at the nucleus.

- The first term contains a ***kinetic energy operator for the motion of each electron*** and the ***Coulomb attraction between the electron and the nucleus***.
- The second term contains the ***electron-electron Coulomb repulsion*** term.
- The equation is not analytically solvable, even for the simplest case, the helium atom for which $N = 2$.

Many-Electron Systems - [Central Field Approximation]

- **Central field approximation (or orbital approximation):**

- We assume that ***each electron moves in the potential of the nucleus plus the averaged potential due to the other N - 1 electrons.***
- Within this model, the Schrödinger equation can be separated into N single electron equations:

$$\left[-\frac{\hbar^2}{2m} \nabla_i^2 + V_i(r_i) \right] \phi_i(\mathbf{r}_i) = E_i \phi_i(\mathbf{r}_i) \text{ where } V_i(r_i) = -\frac{Ze^2}{r_i} + \sum_{j \neq i} \left\langle \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \right\rangle$$

- The solutions of the above equations are known as ***orbitals***. The total wave function would be written as

$$E = \sum_i E_i \quad \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\cdots\phi_N(\mathbf{r}_N)$$

- Within this approximation, each atomic orbital can be written as the product of a radial and an angular function, as to H atom.
 - ▶ The angular part is independent of the other electrons and is therefore simply a spherical harmonic.
 - ▶ However, the radial function is different from that for H atom.
- It provides a useful classification of atomic states and also a starting point.
- It is standard to use the hydrogen atom orbital labels, n , l and m , to label the orbitals. This is called the ***configuration*** of electrons.

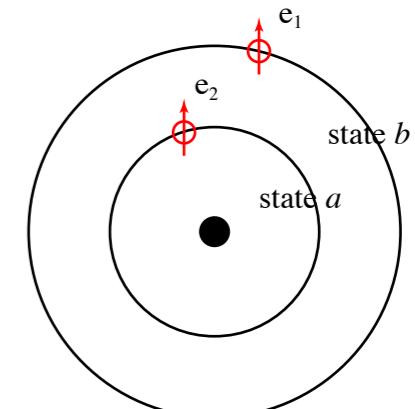
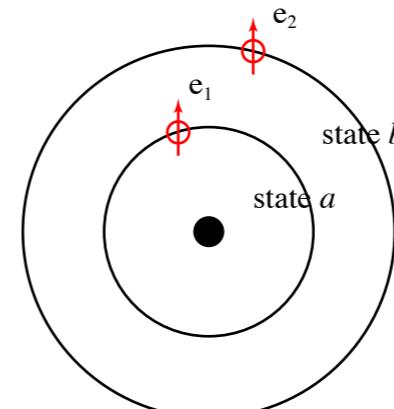
Central Field Approximation: Electron Configuration

- **The configuration** is the distribution of electrons of an atom in atomic **orbitals**.
 - The configuration of an atomic system is defined by specifying the nl values of all the electron orbitals: nl^x means x electrons in the orbital defined by n and l .
 - Each orbital labelled nl actually consists of orbitals with $2l + 1$ different m values, each with two possible values of m_s . Thus the nl orbital can hold a maximum $2(2l + 1)$ electrons.
- **shells, subshells:**
 - Shells correspond with the principal quantum numbers (1, 2, 3, ...). They are labeled alphabetically with letters used in the X-ray notation (K, L, M, ...).
 - Each shell is composed of one or more subshells. The first (K) shell has one subshell, called “1s”; The second (L) shell has two subshells, called “2s” and “2p”.
- **open shell configuration, closed shell configuration:**
 - open shell = shell that is not completely filled with electrons: For instance, the ground state configuration of carbon, which has six electrons: $1s^2 2s^2 2p^2$
 - closed shell = shell of which orbitals are fully occupied: For example, the ground state configuration of neon atom, which has ten electrons: $1s^2 2s^2 2p^6$
- **Active electrons:** As a result of the Pauli Principle, closed shells and sub-shells have both $L = 0$ and $S = 0$. This means that ***it is only necessary to consider ‘active’ electrons, those in open or partially-filled shells.***
- **Equivalent and Nonequivalent Electrons**
 - Nonequivalent electrons are those differing in either n or l values, whereas equivalent electrons have the same n and l values.

[Indistinguishable Particles]

- Consider a system with **two identical particles**. We note that what is physically observable is not a wave function but a probability distribution. This distribution cannot be altered by interchanging the particles. This means that

$$|\Psi(a_1, b_2)|^2 = |\Psi(a_2, b_1)|^2$$



The equation has two possible solutions:

- symmetric solution

$$\Psi(a_1, b_2) = \Psi(a_2, b_1)$$

- antisymmetric solution

$$\Psi(a_1, b_2) = -\Psi(a_2, b_1)$$

Particles 1 and 2 are indistinguishable.

Pauli Exclusion Principle: *Wave functions are antisymmetric with respect to interchange of identical Fermions* (with a half-odd-integer spin). Within the central field approximation, a two-electron wave function which obeys the Pauli Principle can be written

$$\Psi(1, 2) = \frac{1}{\sqrt{2}} [\phi_a(1)\phi_b(2) - \phi_a(2)\phi_b(1)] = -\Psi(2, 1)$$

If the two spin-orbitals are the same ($\phi_a = \phi_b$), then the total wave function is zero, i.e., $\Psi(1,2) = 0$, and no physical (normalizable) state exists. The Pauli exclusion principle is summarized as "**No two electrons can occupy the same spin-orbital state.**"

This exclusion provides the **degeneracy pressure** which holds up the gravitational collapse of white dwarfs and neutron stars.



Wolfgang Ernst Pauli

- **Parity of the wave function**

- The parity of the wave function is determined by how the wave function behaves upon inversion. The square of the wave function, i.e., the probability distribution of the electrons, must be unchanged by the inversion operation.

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \pm \Psi(-\mathbf{r}_1, -\mathbf{r}_2, \dots, -\mathbf{r}_N)$$

- Even parity states are given by “+” sign and odd parity states are given by “−” sign.
- The parity arising from a particular configuration can be determined simply by summing the orbital angular momentum quantum numbers for each of the electrons.
- As closed shells and sub-shells have an even number of electrons, ***it is only necessary to explicitly consider the active electrons.***

$$\text{parity} = (-1)^{l_1+l_2+\dots+l_N}$$

[Electron Configuration - Orbitals]

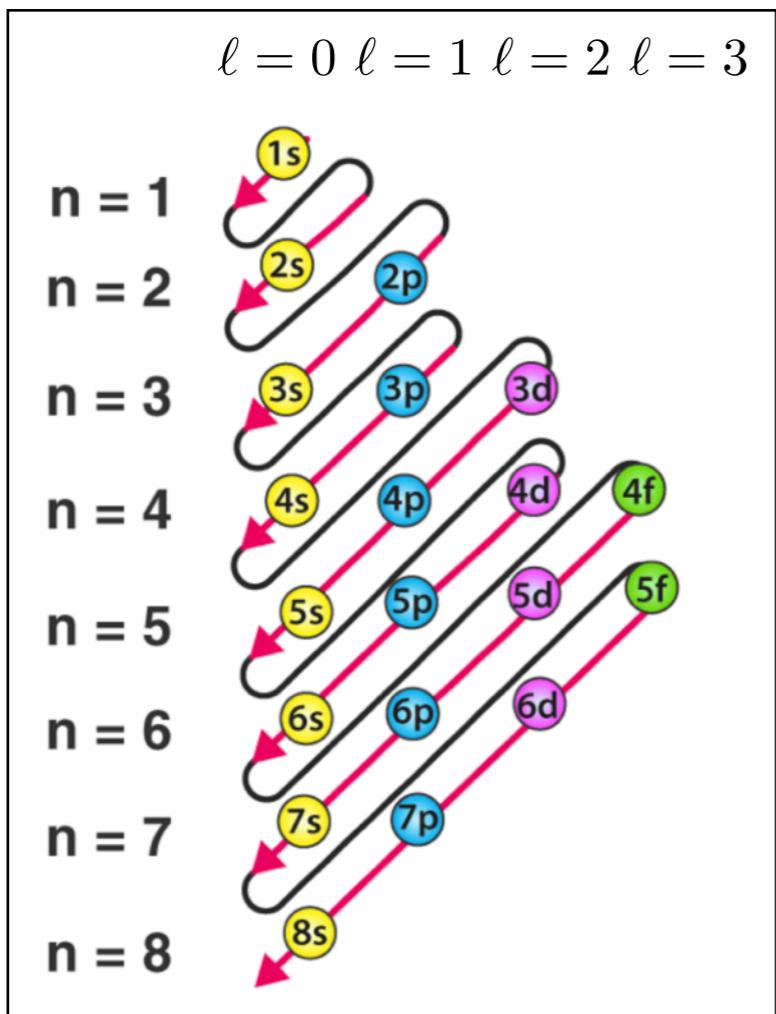
- $n = 1, 2, 3, \dots$: principal quantum number (주양자수)
- $l = 0, 1, 2, \dots, n-1$: orbital angular momentum (quantum number) for each electron (부양자수)

$n = 1, 2, 3, 4, 5 \dots$

$\ell = 0, 1, 2, 3, \dots, n-1 \rightarrow s, p, d, f, g, \dots$

- The electron configuration represents how the electrons are filled in shells and subshells.

$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 \dots$$



Shell (Principle Quantum Number Value)	Subshell (Angular Momentum Quantum Number)	Notation	Maximum Number of electrons
$n = 1$	$l=0$	1s	2
$n = 2$	$l=0$	2s	2
	$l=1$	2p	6
	$l=0$	3s	2
$n = 3$	$l=1$	3p	6
	$l=2$	3d	10
	$l=0$	4s	2
	$l=1$	4p	6
$n = 4$	$l=2$	4d	10
	$l=3$	4f	14

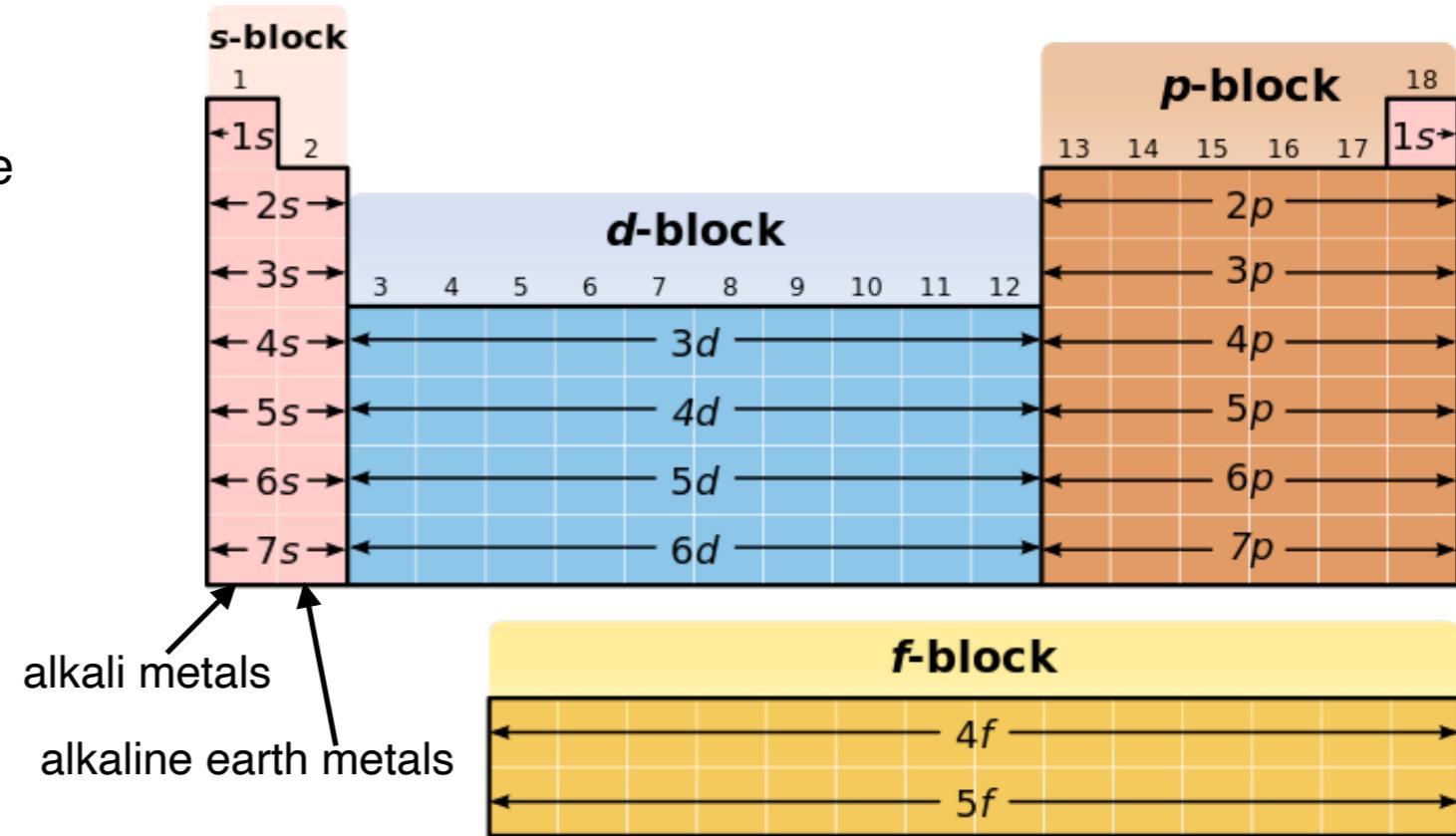
Energy ordering & Periodic Table

- Energy ordering for configuration:**

- For a H atom, the energy of the individual orbitals is determined only by principal quantum number n .
- For complex atoms, the degeneracy on the orbital angular momentum quantum number l is lifted.
- Electrons in low l orbits ‘penetrate’, i.e., get inside orbitals with lower n -values. Penetration by the low l electrons means that they spend some of their time nearer the nucleus experiencing an enhanced Coulomb attraction. This lowers their energy relative to higher l orbitals which penetrate less or not at all.

The orbitals of complex atoms follow a revised energy ordering:

$$E(1s) < E(2s) < E(2p) < E(3s) < E(3p) < E(3d) \simeq E(4s) \dots$$



- Periodic Table**

- The subshell structure of elements up to argon ($Z = 18$) is filled up in a naturally straightforward manner, first according to n and then according to l .
- The $3p$ subshell is all occupied in **argon** (Ar; noble gas) with a closed subshell $3p^6$. The next element **potassium** (K; $Z = 19$), begins by filling in the $4s$, instead of $3d$.

Atom		Z	Configuration
hydrogen	H	1	$1s$
helium	He	2	$1s^2$
lithium	Li	3	K
beryllium	Be	4	K
boron	B	5	K
carbon	C	6	K
nitrogen	N	7	K
oxygen	O	8	K
fluorine	F	9	K
neon	Ne	10	K
sodium	Na	11	K
magnesium	Mg	12	K
aluminium	Al	13	K
silicon	Si	14	K
phosphorus	P	15	K
sulphur	S	16	K
chlorine	Cl	17	K
argon	Ar	18	K
potassium	K	19	K
calcium	Ca	20	K

[LS Coupling]

- The configurations are split into “**terms**” according to the orbital angular momentum **L** and spin angular momentum **S**, and the “terms” are then split into “**levels**” further by the total angular momentum **J**.

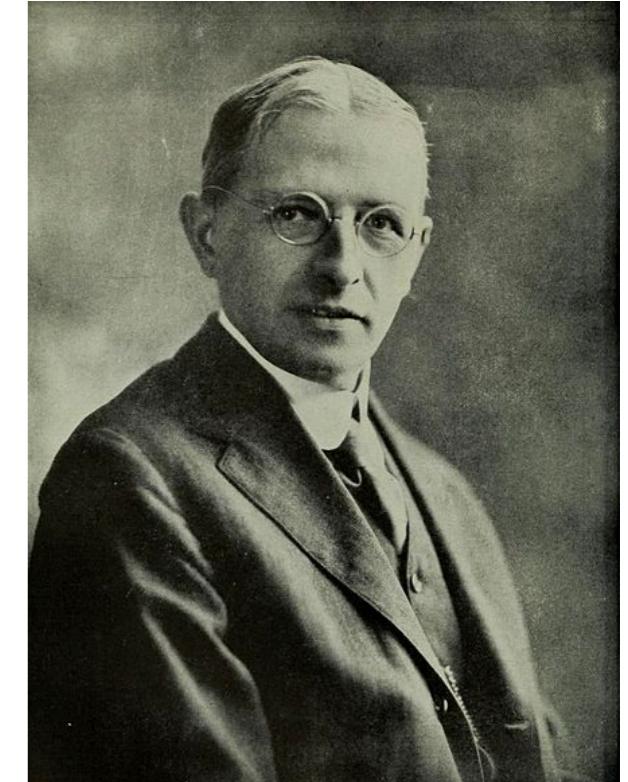
First, add all spin angular momenta for open shells:

$$\mathbf{S} = \sum_i \mathbf{s}_i = \mathbf{s}_1 + \mathbf{s}_2 + \dots$$

Second, add all orbital angular momenta for open shells:

$$\mathbf{L} = \sum_i \mathbf{l}_i = \mathbf{l}_1 + \mathbf{l}_2 + \dots$$

Finally, add the spin angular momentum and orbital angular momentum.



Henry Norris Russell

Hertzsprung-Russell diagram
Russell-Saunders coupling

$$\mathbf{J} = \mathbf{L} + \mathbf{S} \quad \rightarrow \quad J = -|L - S|, -|L - S| + 1, \dots, |L + S| - 1, |L + S|$$

For instance, if $L = 1$ and $S = 1$, then $J = -1, 0, 1$.

Lifting Degeneracy in Configuration: Angular Momentum Coupling, Terms

- There are two coupling schemes or ways of summing the individual electron angular momentum to give the total angular momentum.
- ***L-S coupling (Russell-Saunders coupling):***
 - The orbital and spin angular momenta are added separately to give the total angular momentum \mathbf{L} and the total spin angular momentum \mathbf{S} . These are then added to give \mathbf{J} .

$$\mathbf{L} = \sum_i \mathbf{l}_i, \quad \mathbf{S} = \sum_i \mathbf{s}_i \quad \rightarrow \quad \mathbf{J} = \mathbf{L} + \mathbf{S}$$

- The configurations split into **terms** with particular values of L and S .
- ***j-j coupling***
 - An alternative scheme is to consider the total angular momentum \mathbf{j}_i for each electron by combining \mathbf{l}_i and \mathbf{s}_i and then coupling these \mathbf{j} 's together to give the total angular momentum.

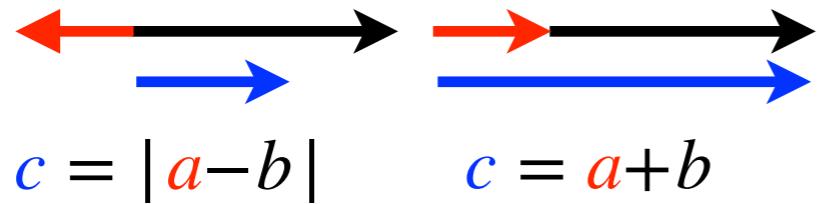
$$\mathbf{j}_i = \mathbf{l}_i + \mathbf{s}_i \quad \rightarrow \quad \mathbf{J} = \sum_i \mathbf{j}_i$$

- Why two coupling schemes?
 - They give the same results for J .
 - For light atoms (lighter than iron), the values of L and S are approximately conserved quantities, and the $L\text{-}S$ coupling scheme is the most appropriate.
 - For heavy atoms (beyond iron), L and S are no longer conserved quantities and $j\text{-}j$ coupling is more appropriate.

Addition of two angular momenta

- In classical mechanics, adding vector a and vector b gives a vector c , whose length must lie in the range

$$|a - b| \leq c \leq a + b \quad \text{Here, } a, b, c \text{ are the lengths of their respective vectors.}$$



- In quantum mechanics, a similar rule applies except that the results are quantized. The allowed values of the quantized angular momentum, c , span the range from the sum to the difference of a and b in steps of one:

$$c = |a - b|, |a - b| + 1, \dots, a + b - 1, a + b$$

- For example, add the two angular momenta $L_1 = 2$ and $L_2 = 3$ together to give $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$. The result is

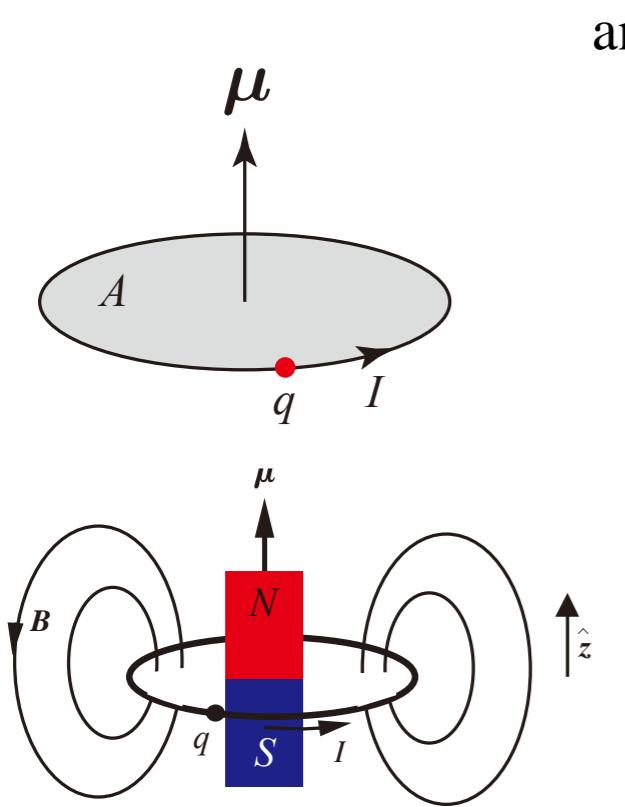
$$L = 1, 2, 3, 4, 5.$$

- Each angular momentum has z -components of. $m = -L, -L + 1, \dots, L, L + 1$.

[Magnetic moments]

- Relation between the magnetic moment and angular momentum

Consider a charge q with mass m that orbits in a circle at radius r about the z -axis with angular velocity ω .



angular momentum

$$\begin{aligned} \mathbf{J} &= \mathbf{r} \times \mathbf{p} \\ &= r \times (mv)\hat{\mathbf{z}} \\ &= mr^2\omega\hat{\mathbf{z}} \end{aligned}$$

magnetic momentum

$$\begin{aligned} \mu &= IA\hat{\mathbf{z}} \\ \text{current } I &= \frac{dq}{dt} = \frac{q}{P} = \frac{q\omega}{2\pi} \\ \text{area } A &= \pi r^2 \\ \mu &= \frac{1}{2}q\omega r^2\hat{\mathbf{z}} \end{aligned}$$

↑
period $P = \omega/2\pi$

Consequently, the classical relation between magnetic moment and angular momentum for an orbiting charge is

$$\mu = \frac{q}{2m}\mathbf{J}$$

Now consider a spinning sphere with uniform mass and charge distributions. It consists of many orbiting charge and mass elements, each obeying the above equation. Thus, the equation is also valid for the entire sphere.

In quantum mechanics, **the magnetic moment of the electron**, which is a point charge with zero radius, is given by

$$\boldsymbol{\mu}_e = -g_e \frac{e}{2m_e} \mathbf{S} \quad (\text{where } g_e = 2.0 \text{ in Dirac equation})$$

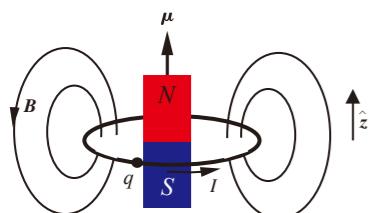
The magnetic moment of the electron is opposed to the direction of the spin \mathbf{S} , because of the negative charge.

Magnetic dipole in a magnetic field

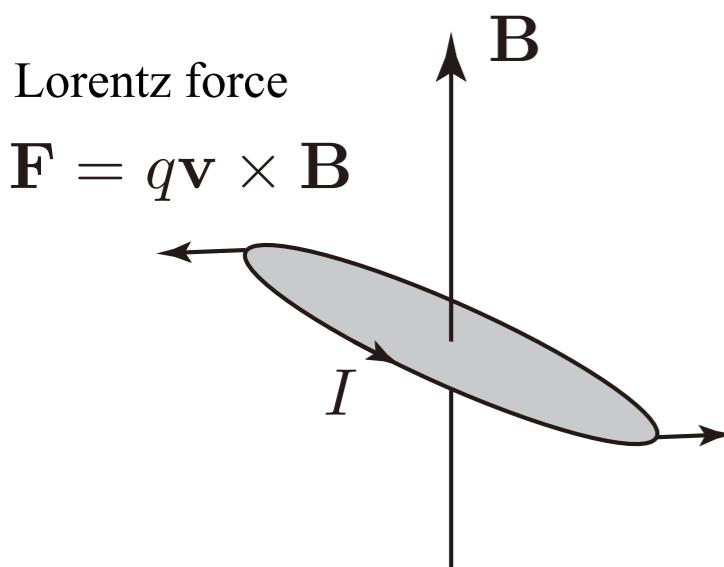
- A magnetic dipole will tend to align with an external magnetic field just as a compass needle aligns itself with the magnetic field of the earth.

One can visualize the external field acting on a magnet. This magnet experiences a torque tending to align it with the \mathbf{B} field.

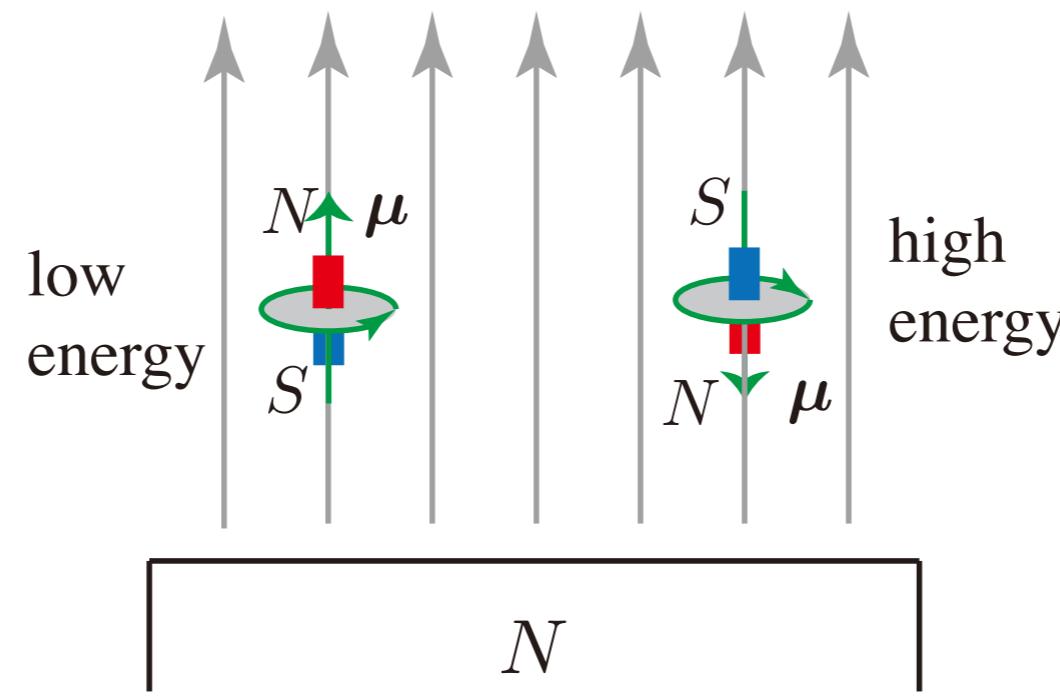
Integration of this torque over the appropriate angles yields a potential energy that is a function of the angle θ between the magnetic field \mathbf{B} and magnetic moment μ vector. The lowest potential energy occurs when the two vectors are aligned. The potential energy E_{pot} turns out to be the negative dot product of the vectors μ and \mathbf{B} :



$$E_{\text{pot}} = -\mu \cdot \mathbf{B} = -\mu B \cos \theta$$



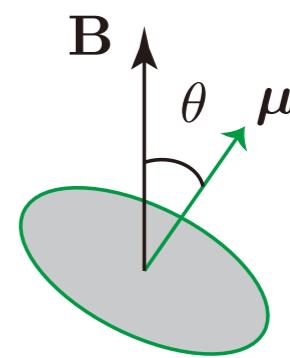
$$\text{torque } \tau = \mathbf{r} \times \mathbf{F}$$



N

$$E_{\text{pot}} < 0 \quad \text{if } \theta < \frac{\pi}{2}$$

$$E_{\text{pot}} > 0 \quad \text{if } \theta > \frac{\pi}{2}$$



$$E_{\text{pot}} = -\mu \cdot \mathbf{B}$$

[Spin-Orbit Coupling]

- The fact that the remaining spin-orbit splitting is much smaller makes the LS coupling scheme a very useful one.
- **Fine-structure splitting:** Relativistic effects couple electron orbital angular momentum and electron spin to give the so-called fine structure in the energy levels. Inclusion of relativistic effects splits the **terms** into **levels** according to their J value.
- When the electron will move around the nucleus with a non relativistic velocity \mathbf{v} , the electric field exerting on the electron will be $\mathbf{E} = Ze\frac{\mathbf{r}}{r^3}$. (Note that the nucleus has a positive charge Ze .)

In the electron rest frame, this electric field will be perceived as a magnetic field

$$\begin{aligned}\mathbf{B}' &= \mathbf{B}'_{\perp} = \gamma(\mathbf{B}_{\perp} - \boldsymbol{\beta} \times \mathbf{E}) = -\frac{\mathbf{v}}{c} \times \mathbf{E} \\ &= -\frac{Ze}{c} \frac{\mathbf{v} \times \mathbf{r}}{r^3} \\ &= \frac{Ze}{m_e c r^3} \mathbf{L} \quad (\mathbf{L} = \mathbf{r} \times \mathbf{p})\end{aligned}$$

Here, the magnetic field is perpendicular to the electron's orbital plane.

(where $\mathbf{L} \equiv \mathbf{r} \times \mathbf{p} = m_e \mathbf{r} \times \mathbf{v}$ is the electron's orbital angular momentum)

- This magnetic field will interact with the electron's **magnetic moment**, which is

$$\boldsymbol{\mu}_e = -\frac{e}{m_e} \mathbf{S}$$

- Then, the interaction energy is

$$U = -\boldsymbol{\mu} \cdot \mathbf{B} = \frac{Ze^2}{m_e^2 c^2 r^3} \mathbf{S} \cdot \mathbf{L}$$

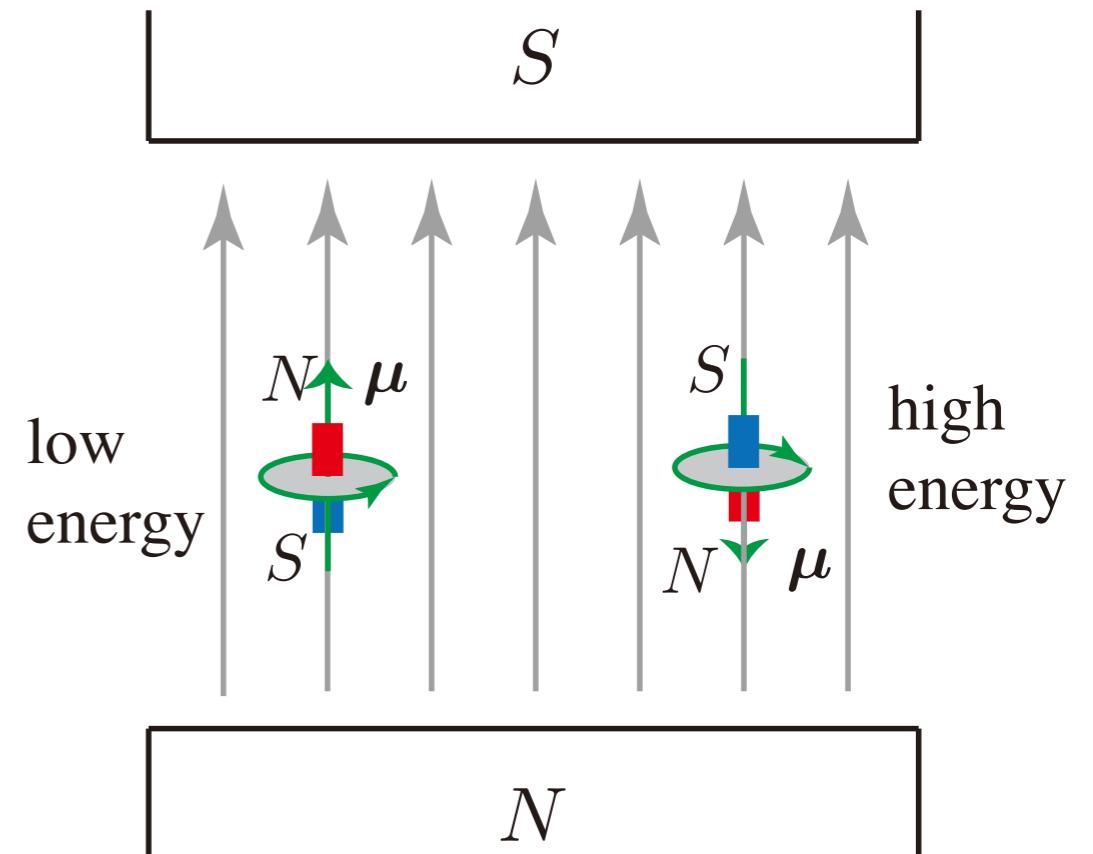
- For the sum of the interactions of all electrons will be

$$H_{\text{so}} = \xi (\mathbf{S} \cdot \mathbf{L})$$

From the relation $\mathbf{J}^2 = |\mathbf{L} + \mathbf{S}|^2 = \mathbf{L}^2 + \mathbf{S}^2 + 2\mathbf{S} \cdot \mathbf{L}$,

we obtain

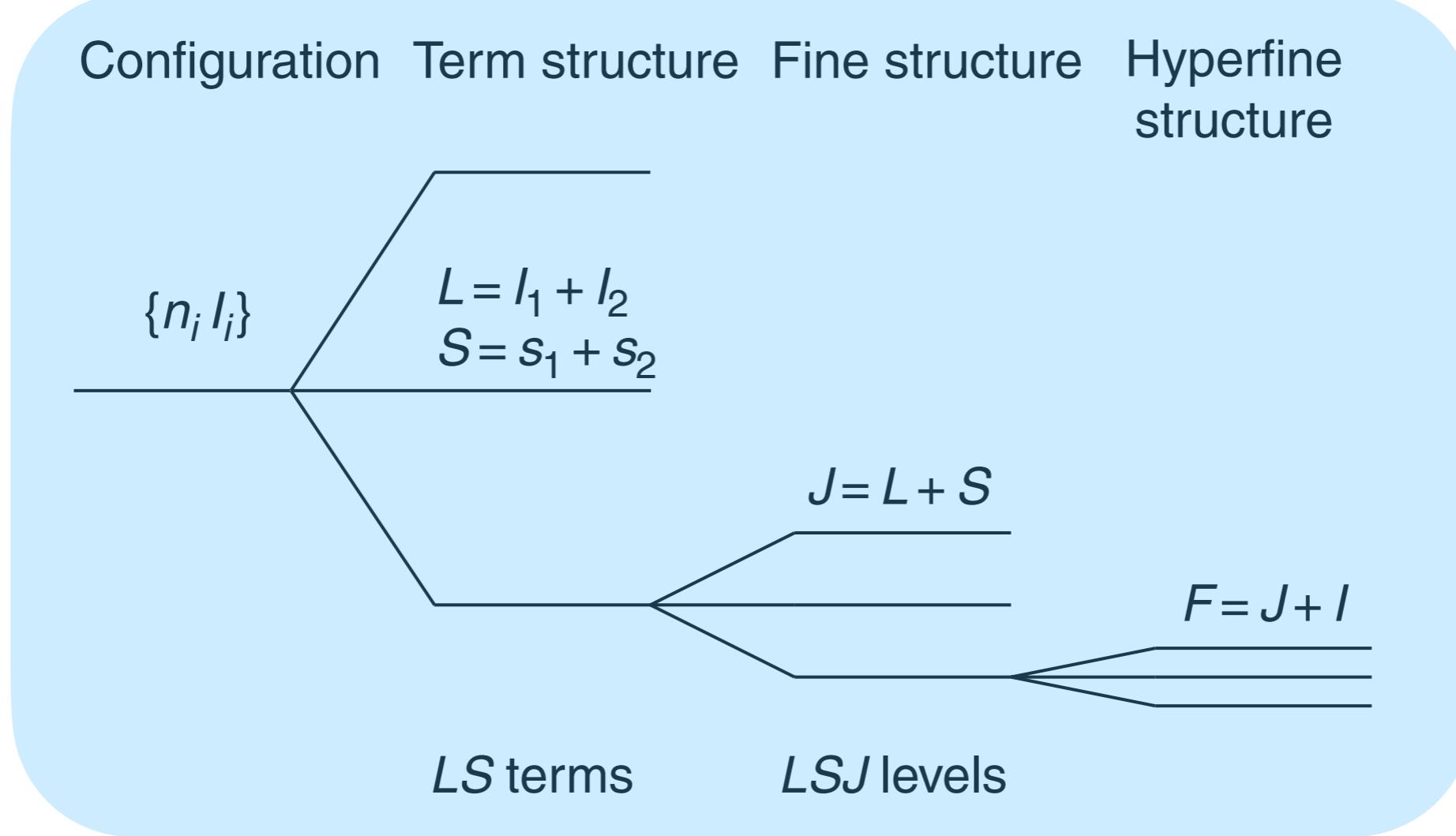
$$H_{\text{so}} = \frac{1}{2}\xi (\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2)$$



The eigen energy of the operator is given by $E_{\text{so}} = \frac{1}{2}C [J(J+1) - L(L+1) - S(S+1)]$.

The states split into several J levels for a given S and L .

- Electronic configuration and energy level splitting
 - Configurations \Rightarrow Terms \Rightarrow Fine Structure (Spin-Orbit Interaction) \Rightarrow Hyperfine Structure (Interaction with Nuclear Spin)

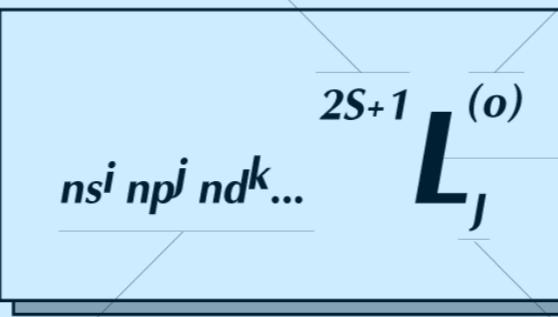


[Spectroscopic Notation]

- Spectroscopic Notation

Total Term Spin Multiplicity:
 S is vector sum of electron spins ($\pm 1/2$ each)
 Inner full shells sum to 0

Term Parity:
 o for odd, nothing for even



Total Term Orbital Angular Momentum:
 Vector sum of contributing electron orbitals.
 Inner full shells sum to 0.

Electronic Configuration:
 the electrons and their orbitals
 (i.e. $1s^2 2s^2 3p^1$)

The Number of levels in a term is the smaller of $(2S+1)$ or $(2L+1)$

Total Level Angular Momentum:
 Vector sum of L and S of a particular level in a term.

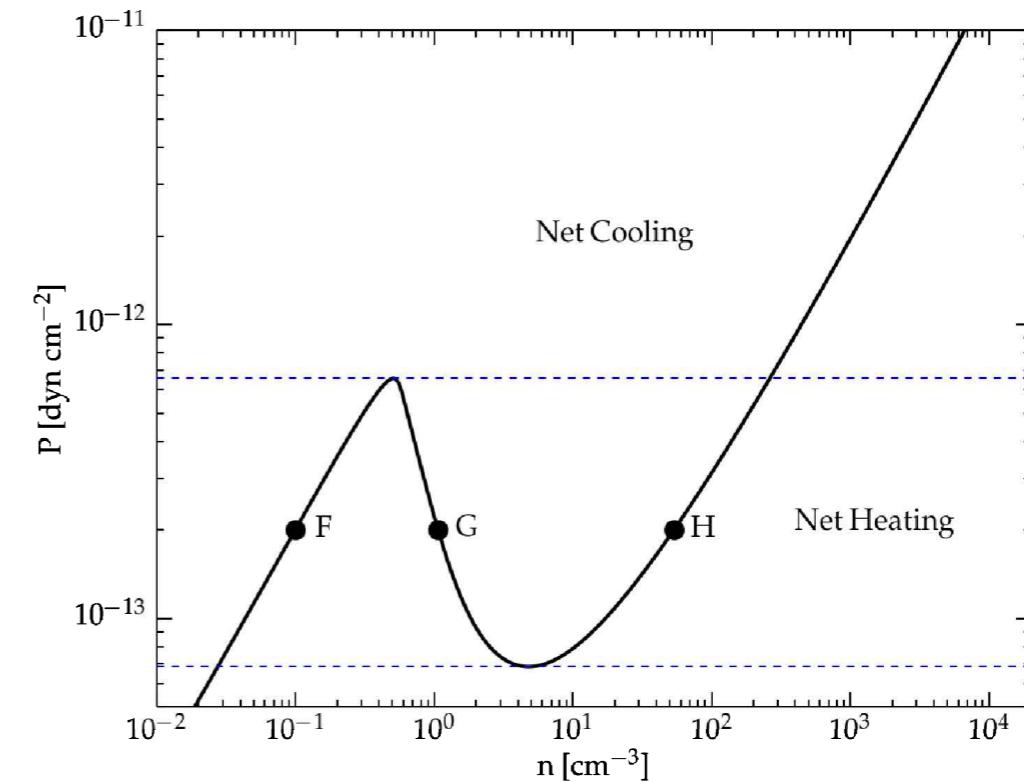
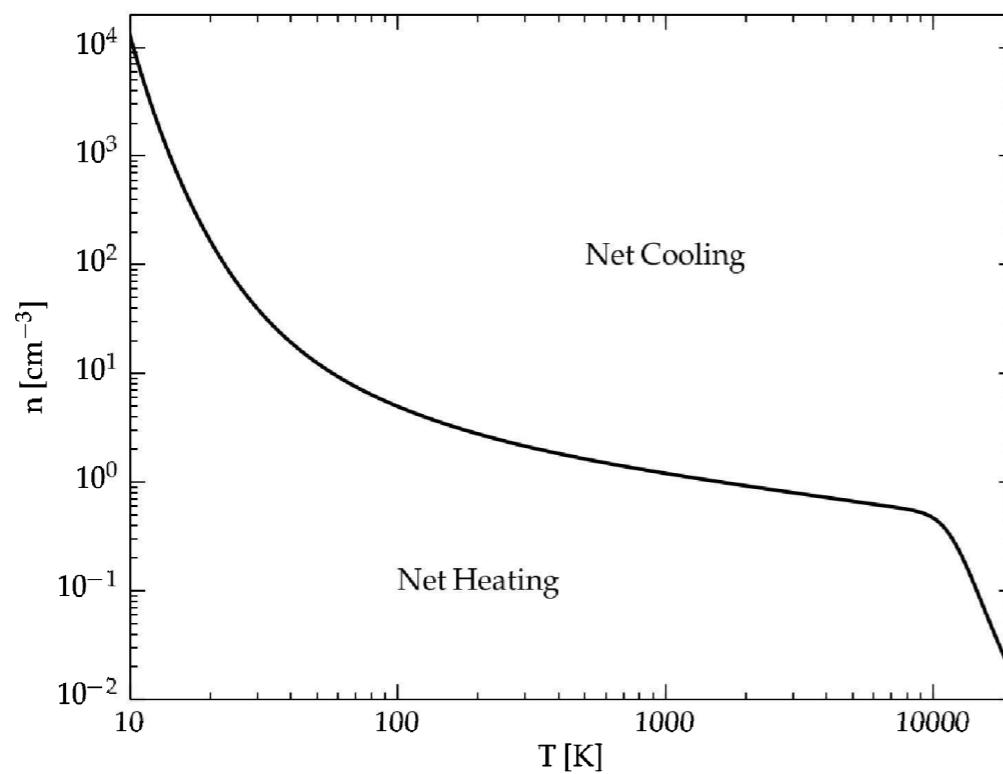
- A state with $S = 0$ is a ‘singlet’ as $2S+1 = 1$.
 - ▶ $J = L$ (singlet)
- A state with $S = 1/2$ is a ‘doublet’ as $2S+1 = 2$
 - ▶ $J = L - 1/2, L + 1/2$ (doublet if $L \geq 1$)
- One with $S = 1$ is a ‘triplet’ as $2S+1 = 3$
 - ▶ $J = L - 1, L, L + 1$ (triplet $L \geq 1$)

shells	$n = 1, 2, 3, 4, 5 \dots$
subshells	$\ell = 0, 1, 2, 3, 4 \dots \rightarrow s, p, d, f, g, \dots$
terms	$L = 0, 1, 2, 3, 4 \dots \rightarrow S, P, D, F, G, \dots$
sharp, principal, diffuse, fundamental, ...	

Homework (due date: 04/03)

[Q2] Two stable phases

- Use the formulae for the photoelectric heating rate by dust and the cooling rate by [CII] 158 μm , [OI] 63.2 μm , and Ly α , described in this lecture note (and textbook).
 - Use python or whatever you can use.
1. Reproduce the figures shown below.



2. Make a plot “P versus T,” in addition to the above plots.
3. Compute the numerical values of the “**stable**,” equilibrium **densities** and **temperatures** for two pressures $P = 2 \times 10^{-13} \text{ dyn cm}^{-2}$ and $4 \times 10^{-13} \text{ dyn cm}^{-2}$.