Notes for Diffuse Matter in Space
UC Santa Cruz, Fall 2023

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Diffuse Matter in Space **Fall 2023**

Lecture 1: Introduction

Lecturer: Nia Imara *28 September* *Aditya Sengupta*

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Note: *LaTeX format adapted from template for lecture notes from CS 267, Applications of Parallel Computing, UC Berkeley EECS department.*

Diffuse matter = ISM + IGM, we may use "ISM" as a catch-all term but most of it applies to both.

Overdensities in the magnetic field plot: correspond to star-forming regions like the LMC.

The JWST picture of the Carina Nebula shows us dust is more opaque in the optical than the IR; we see a lot more structure in IR imaging. With JWST we can see stars and proto-stellar jets.

We also want to develop an idea of what's happening outside our galaxy. Imaging other galaxies (M82, M33) at multiple wavelengths can show us star-forming regions. The LMC and SMC are two of the largest dwarf galaxies to the Milky Way.

For lecture 2: bring in one image of something ISM or IGM related, read a little about it, email Nia by 5pm on Monday.

Our conception of the ISM has been very closely tied to how we've been able to observe it, since we started looking at the sky. It's evolved through naked-eye observing, photographic plates, spectroscopy (which gives us chemistry and kinematics), radio astronomy (detailed imaging of mostly-cold and mostly-dark regions), UV/X-ray/IR space-based observatories, and interferometry.

In the early 1800s, astronomers began to recognize that there is material between the stars. The discovery of the ISM and developing an understanding of its underlying physics are relatively recent. William Herschel and Charles Messier separately started cataloguing objects (the NGCs and the Ms). William and Caroline Herschel cataloged dark clouds and published a paper discussing 'holes' in the sky in 1786.

In 1919, Edward Barnard published a catalogue of 182 dark objects, and theorized these were evidence of "masses of obscuring matter" in space. In 1904, Hartmann showed narrow, stationary absorption lines in the spectrum of the binary star δ Orionis, which didn't move with the redshifting/blueshifting of the star that's evident in other lines. He concluded those lines must have been produced by a cloud between the star and us. These turned out to be calcium lines.

In the 1930s, Robert Trumpler observed star clusters and compared the distance that should be expected from their size and brightness to the actual distance, and his observations suggested distant things look both smaller and fainter than they should be. This suggests the presence of obscuring material that's widespread, which suggests it is not a local phenomenon. He suggested cosmic dust may cause this.

In the early 1900s, balloon flights at higher than 5km up found ionizing radiation that increases with altitude, and a flight during a solar eclipse argued they had an interstellar origin. In 1927, we found that these cosmic rays were high-energy charged particles.

The 1940s and 1950s saw the development of quantum mechanics, radio astronomy, and radar technology. Hendrik van de Hulst predicted the existence of the HI 21cm line, and Ewen and Purcell observed it with a radio telescope. Cold HI emitting at 21cm makes up most of the mass of ISM gas in the Milky Way ($4 \times 10^9 \mathrm{M}_\odot$.)

In 1966, Lynds and Stockton observed absorption lines in spectra toward QSOs and discovered the Lyman-alpha forest: a dense collection of hydrogen absorption lines that don't match any other wavelength. We

see a forest because light passes through a large number of hydrogen clouds at various redshifts.

Radio observations enabled the discovery of interstellar molecules in the 1960s-1970s. Jefferts, Penzias, and Wilson observed the 2.6mm rotational line of CO, and realized almost as much mass is traced out by CO as HI.

Space astronomy enabled us to observe γ-rays, X-rays, and UV and IR light. This lets us observe interstellar dust both in extinction and emission. IRAS (1983) was the first space-based astronomy IR detector, and it let us see that emission from dust extinction in the IR correlated to dark patches in the optical. Rosat (1990) produced the first sensitive all-sky image in x-rays.

In the 1990s, ground-based interferometers and radio imaging were expanded, culminating in ALMA.

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Lecture 2: Overview of the ISM

Lecturer: Nia Imara	*3 October*	*Aditya Sengupta*

The ISM consists of gas, dust, photons, magnetic fields, cosmic rays, and dark matter. Dark matter makes up the bulk of the mass but isn't super significant for us in this class. In the Milky Way, we have about $10^{12} M_\odot$ of mass in dark matter, $10^{11} M_\odot$ in stellar mass, and $6 \times 10^9 M_\odot$ in the ISM.

The usual dust-to-gas ratio we use in the Milky Way is 1/100. Gas and dust are well correlated in the disk of the Milky Way, but theratio can and does vary. There are average temperatures of 10-20K. There are small sub-μm size grains, which we can tell from reddening (Mie?). Dust is mostly composed of C, O, Fe, Si, and Mg. These elements are the byproduct of dying stars.

Cosmic rays are very energetic particles pervading the ISM. Cosmic rays are mostly protons, but they can also be other nuclei and electrons at relativistic speeds. We'll usually see energies of about 1 eV per cubic centimeter in the ISM.

The average interstellar radiation fields varies spatially. The main contributions are from starlight in the optical, reradiation from the dust in the IR, and from the CMB in the radio.

Magnetic fields pervade the interstellar medium, and we notice they're closely tied to the gas. This arises from the partial ionization of the gas in the ISM, which means we have free electrons; if they're moving, this induces magnetic fields. The energy density here as well is about 1 eV per cubic centimeter.

In the Milky Way, gas is 99% of the ISM mass. About 23% of this is ionized, 60% is neutral, and 17% is molecular. Depending on their temperatures and densities, there are about six phases. We'll use H I for atomic hydrogen, H II for ionized hydrogen, and H_2 for molecular hydrogen. Density scales about inversely with the fraction of volume taken up in the ISM.

It's notable that the ISM has many components that all have the same order-of-magnitude energy density, which means there's rarely a dominant factor. This is compounded by the huge dynamic ranges in density and temperature. Very dense regions of the ISM are "ultra-high" vacuum, so it's hard to reproduce those conditions in a lab. Most processes are not in thermodynamic equilibrium because of the low density, and there are feedback loops between different processes.

We'll get a sense for the numbers involved in the main processes. To start with, we'll get some order of magnitude estimates of the densities of gas and dust in the Milky Way. Assume $M_N \simeq 4 \times 10^9 M_\odot$, distributed uniformly in a disk with $R = 15$ kpc and height 200 pc. Assume the ratio He/H = 0.1. First, let's ask: what's the average number density of hydrogen nuclei in the disk? We can get this by computing $\frac{\text{total mass}}{1.4 m_H \times \text{volume of disk}}$, where the disk volume comes from $V = \pi R^2 H$ and the factor of 1.4 comes from the helium abundance. This gives us a density of 0.82cm^{-3}.

Next, we can calculate the number density of dust. If 0.7% of the interstellar mass is in the form of dust, the radius of a dust grain is $a = 0.1\mu$m, and the density is 2g/cm^3, we can get a number density by taking

$$n_d = \frac{M_{\text{dust}}/m_d}{V_d} = \frac{0.007 M_N/\rho_d \cdot \frac{4}{3}\pi a_d^3}{V_d} \tag{2.1}$$

We get $n_d = 1.6 \times 10^{-12} \text{cm}^{-3}$.

Next, we'll ask about the optical depth due to dust. To be more specific, we'll measure the optical depth from us to the galactic center, 8.5 kpc away. We'll use $\tau_d = n_d \sigma_d L$. We calculated n_d just now, and we'll say $\sigma_d = C_{\text{ext}}$; there's a few different cross-sections we could use, so we want to be specific that this is the one for extinction. We'll define $Q_{\text{ext}} = \frac{C_{\text{ext}}}{C_{\text{geom}}}$ and we'll say it's equal to 1 this time just to make it easy. The geometric cross-section is $C_{\text{geom}} = \pi a_d^2$. We have

$$\tau_d = n_d \pi a_d^2 R_{\text{disk}} = 13.2. \tag{2.2}$$

We get an extinction of

$$A_v = \frac{2.5}{\ln 10} \tau = 1.086\tau, \tag{2.3}$$

so we see $A_v = 14.3$ mag of visual extinction. So even though dust is only 1% of the overall mass of the ISM, it causes a lot of extinction!

Finally, we'll (). 30% of gas and dust are contained within molecular clouds of a radius of about 15 pc and a number density $n_{\text{H}_2} = 100 \text{cm}^{-3}$. We can use this to calculate the number of molecular clouds in the galaxy, which comes out to about 10^4; this matches observations to order of magnitude.

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	Lecture 3: Collisional processes	
Lecturer: Nia Imara	*5 October*	*Aditya Sengupta*

Today we'll:

1. Develop a theory for collisions

2. Derive the collision rate coefficient

3. Apply this to three basic types of collisions in the ISM.

In the materials we're used to, collisions occur so frequently that we assume material reaches thermodynamic equilibrium, but that's not necessarily true in the ISM. Collisions can govern

- Energy distribution among particles in the gas

- Collisional excitation

- Recombination

- Collisional excitation

- Chemical reactions

- Gas-dust grain collisions

- Grain-grain collisions

- ...

Before we study any of this, we have to calculate collisional rates that don't depend on thermodynamic equilibrium.

In general, a collisional process occurs when particles A and B collide and lead to some products. The products can be many different things: we can have elastic collisions, with $A + B \rightarrow A + B$ (particles exchange momentum); inelastic collisions, where (e.g.) $A^* + B \rightarrow A + B^*$ (particles undergo internal energy changes, the asterisks represent an excited state); and chemical reactions, where (e.g.) $A + B \rightarrow C$.

A cross-section σ_A moving at velocity v_A will sweep up particles at a rate $\sigma_A v_A$. If these collide with particles B that have very small cross-sections, the number of collisions of A with B is $n_B \sigma_A v_A$. To make this more general, we can say that the collective cross-section for this collision is σ_{AB}, and that the velocity of A relative to B is v_{AB}. This gives us the number of collisions per second per unit volume,

$$\text{number of collisions per second per unit volume} = n_A n_B \sigma_{AB} v_{AB}. \tag{3.1}$$

This assumes that all the particles have the same velocity v_{AB}. In fact, particles follow Maxwellian distributions; even in the ISM, we usually have enough density and enough of a fraction of elastic collisions to maintain this.

$$f_v \mathrm{d}v = 4\pi \left(\frac{\mu}{2\pi kT} \right)^{3/2} \exp \left(\frac{-\mu v^2}{2k_B T} \right) v^2 \mathrm{d}v. \tag{3.2}$$

This is a pdf, so we can integrate over it to find the number density per range of velocities. Here, $\mu = \frac{m_A m_B}{m_A + m_B}$ is the reduced mass.

Next, we want to find a reaction rate per unit volume. We'll say we're interested in the *two-body collisional rate coefficient*, $\langle \sigma v \rangle_{AB}$.

$$\langle \sigma v \rangle_{AB} = \int_0^\infty v f_v \sigma_{AB}(v) \mathrm{d}v \equiv k_{AB}. \tag{3.3}$$

Here, $\sigma_{AB}(v)$ is the velocity-dependent interaction cross-section. In more probabilistic terms, we're interested in the quantity $E[v\sigma_{AB}]$, which makes sense based on the notation. Note that the units of $\langle \sigma_v \rangle$ are volume per unit time.

Now, plugging in f_v, we get

$$k_{AB} = \int_0^\infty v\sigma_{AB}(v) \times 4\pi \left(\frac{\mu}{2\pi k_B T} \right)^{3/2} \exp \left(\frac{-\mu v^2}{2k_B T} \right) v^2 \mathrm{d}v \tag{3.4}$$

$$= 4\pi \left(\frac{\mu}{2\pi k_B T} \right)^{3/2} \int_0^\infty v^3 \sigma_{AB}(v) \exp \left(\frac{-\mu v^2}{2k_B T} \right) \mathrm{d}v \tag{3.5}$$

$$\tag{3.6}$$

To simplify this, let's do a change of variables to energy: $E = \mu v^2 / 2$, $\mathrm{d}E = \mu v \, \mathrm{d}v$. Further, let $x = \frac{E}{k_B T}$, $\mathrm{d}x = \frac{\mathrm{d}E}{k_B T} = \frac{\mu v}{k_B T} \mathrm{d}v$. Carrying out the change of variables, we get

$$k_{AB} = \sqrt{\frac{8k_B T}{\pi \mu}} \int_0^\infty x e^{-x} \sigma_{AB}(x k_B T) \mathrm{d}x. \tag{3.7}$$

We'll be considering three types of collisions in this class:

1. Neutral-neutral ("hard sphere") collisions

2. Charged-neutral particle collisions

3. Charged-charged particle collisions.

This is in increasing order of how important the long range forces between the particles are in the collision.

We'll start with hard sphere collisions. Imagine two particles with different radii, r_A and r_B. (You can calculate collision rate coefficients for three- and more-body collisions, but these are vanishingly rare in the ISM.) The cross-section is $\sigma_{AB} = \pi(r_A + r_B)^2$, which we get by combining their radii center to center.

We note that σ_{AB} is independent of velocity, so we can pull it out of the integral, and we're left with

$$k_{AB} = \sigma_{AB}\sqrt{\frac{8k_B T}{\pi \mu}} \int_0^\infty x e^{-x} \mathrm{d}x = \sigma_{AB}\sqrt{\frac{8k_B T}{\pi \mu}}. \tag{3.8}$$

Overall, we get $k_{AB} \propto T^{1/2}$.

Let's plug in some numbers to get a sense for things. Suppose both particles have a radius of 1Å. Then we get

$$k_{AB} = 1.81 \times 10^{-10} \left(\frac{T}{100\mathrm{K}}\right)^{1/2} \left(\frac{\mu}{m_H}\right)^{-1/2} \left(\frac{r_A + r_B}{2\mathrm{\mathring{A}}}\right)^2 \mathrm{cm}^3 \mathrm{s}^{-1}. \tag{3.9}$$

For charged-neutral collisions, imagine a particle with a charge Ze. The neutral polarized atom experiences an attractive force,

$$F = -\frac{2\alpha Z^2 e^2}{r^5}. \tag{3.10}$$

Here, α is the polarizability of the neutral particle. It's usually on the order of a_0^3, where $a_0 = 5.292 \times 10^{-9}$ cm is the Bohr radius.

We can integrate this force with respect to $\mathrm{d}r$ to get an interaction potential:

$$U(r) = -\frac{1}{2}\frac{\alpha Z^2 e^2}{r^4}. \tag{3.11}$$

We can define a critical impact parameter, b_0, which is the distance of closest approach for the particle to travel undeflected. At this point, we can say $U(b_0) = -\frac{E_{cm}}{4}$, and we'll use this to solve for b_0.

$$-\frac{E_{cm}}{4} = -\frac{1}{2}\frac{\alpha Z^2 e^2}{r^4} \implies b_0 = \left(\frac{2\alpha Z^2 e^2}{E_{cm}}\right)^{1/4}. \tag{3.12}$$

Substituting in some typical numbers, we get

$$b_0 = 6.62 \times 10^{-8} Z^{1/2} \left(\frac{\alpha}{\alpha_H}\right)^{1/4} qty(\frac{0.01\mathrm{eV}}{E_{cm}})^{1/4} \mathrm{cm}. \tag{3.13}$$

Here, $\alpha_H = 4.5a_0^3$ is the polarizability of neutral hydrogen. Also note that b_0 is generally much larger than the radii of the particles involved. Taking $\sigma_{AB} = \pi b_0^2$ and substituting into the same integral as before, we get

$$k_{AB} = 2\pi Z e \sqrt{\frac{\alpha}{\mu}} = 8.98 \times 10^{-10} Z \left(\frac{\alpha}{a_0^3}\right)^{1/2} \left(\frac{\mu}{m_H}\right)^{-1/2} \text{cm}^3\text{s}^{-1}. \tag{3.14}$$

In charged-charged collisions, long-range forces are not negligible, and non-negligible transfer of momentum is possible.

We'll make the impact approximation, where we assume a projectile moves in a straight line act constant speed. We neglect changes in particle velocities during the encounter. We'd like to calculate the change in transverse momentum experienced by the projectile particle.

When the angle between the particles is θ, the distance between them is $\frac{b}{\cos\theta}$. The total force is

$$F = \frac{Z_1 Z_2 e^2}{(b/\cos\theta)^2} \tag{3.15}$$

so the total perpendicular force is

$$F_\perp = \frac{Z_1 Z_2 e^2}{b^2} \cos^3\theta. \tag{3.16}$$

Recall that $F = \frac{\mathrm{d}p}{\mathrm{d}t}$. The total momentum transfer is obtained by

$$\Delta p_\perp = \int_{-\infty}^{\infty} F_\perp \mathrm{d}t. \tag{3.17}$$

We switch units: $\mathrm{d}t \to \mathrm{d}\theta$. We know that $x = b\tan\theta$, so $\mathrm{d}\theta = \frac{v_1}{b}\cos^2\theta \mathrm{d}t$. Integrating over time, we get

$$\Delta p_\perp = \int_{-infty}^{\infty} F_\perp \mathrm{d}t = \frac{Z_1 Z_2 e^2}{b^2} \int_{-\infty}^{\infty} \cos^3\theta \mathrm{d}t = \frac{2Z_1 Z_2 e^2}{b v_1}. \tag{3.18}$$

So how can we use this to tell us about σ_{AB} and k_{AB}?

Consider an atom or ion with a single bound electron. Let I be the energy required to ionize it. Consider another high-speed electron passing by this charged particle ($KE \gg I$). Below a certain impact parameter, the electron passing by is sufficiently close for sufficiently long to ionize the particle.

The kinetic energy is $KE = \frac{\Delta p^2}{2m_e}$. We need this to be greater than the ionization energy, and we can work out the critical impact parameter at which this happens:

$$\frac{\Delta p^2}{2m_e} > I \implies b < \sqrt{\frac{2Z_{\text{particle}}^2 e^4}{m_e v_e^2 I}} = b_{\max}. \tag{3.19}$$

We can use this to find the cross-section: $\sigma(v) \approx \pi b_{\max}^2 = \frac{2\pi Z_p^2 e^4}{m_e v_e^2 I}$. Assuming this applies down to the minimum impact velocity for which it's energetically possible to ionize the atom, we can translate this into a minimum velocity: $v_{\min} = \left(\frac{2I}{m_e}\right)^{1/2}$. We can work out a rate for collisional ionization:

$$k_{AB} = Z_p^2 \left(\frac{8\pi}{m_e k_B T}\right)^{1/2} \frac{e^4}{I} \exp\left(-\frac{I}{k_B T}\right). \tag{3.20}$$

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Lecture 4: Statistical mechanics	
Lecturer: Nia Imara *10 October* *Aditya Sengupta*	

Today, we'll be talking about

1. Fluid behaviour

2. The law of mass action

3. The principle of detailed balance

4.1   Fluid behaviour

First, consider a collection of particles. Under what conditions can we talk about it being a fluid, and about it having a single temperature? At a large volume, we want to talk about a single bulk velocity and a single temperature. Our goal for now is going to be to figure out a scale at which we can start talking about these collective properties.

Our first case will be talking about neutral particles. We can consider a collection of neutral particles to be a fluid on scales much greater than the fluid's mean free path.

$$\lambda_{\mathrm{mfp}} = \frac{1}{n\sigma}. \tag{4.1}$$

For typical values of the ISM we get

$$\lambda_{\mathrm{mfp}} = 55 \left(\frac{r}{1\text{Å}}\right)^{-2} \left(\frac{n}{1\text{cm}^{-3}}\right)^{-1} \text{AU}. \tag{4.2}$$

For a population containing particles at very disparate masses, this gets more complicated because each interaction won't have as significant of a change in momentum.

The more complicated case involves charged particles. Consider a particle with charge $Z_1 e$ moving through a field of particles with charge $Z_2 e$. The change in momentum under the impulse approximation is

$$\Delta p_\perp = \frac{2Z_1 Z_2 e^2}{b v_1}. \tag{4.3}$$

On average, the change in momentum will be zero, but the RMS momentum change won't be zero, because of directional effects. The rate at which the RMS of $\Delta p_\perp$ increases is

$$\langle \frac{\mathrm{d}}{\mathrm{d}t}(\Delta p_\perp)^2 \rangle = (\text{encounter rate for particle 1}) \times (\Delta p_\perp)^2. \tag{4.4}$$

The differential rate of encounters with impact parameter b is given by $n_2 v_1 \times 2\pi b \mathrm{d}b$. This tells us

$$\langle \frac{\mathrm{d}}{\mathrm{d}t}(\Delta p_\perp)^2 \rangle = \int_{b_{\min}}^{b_{\max}} n_2 v_1 2\pi b \left(\frac{2Z_1 Z_2 e^2}{b v_1} \right) \mathrm{d}b = \frac{8\pi n_2 Z_1^2 Z_2^2 e^4}{v_1} \int_{b_{\min}}^{b_{\max}} \frac{\mathrm{d}b}{b}. \tag{4.5}$$

This diverges if we let $b_{\min} \to 0$ or $b_{\max} \to \infty$, so we need to pick reasonable limits. For $b_{\min}$, we'll pick the point at which the impulse approximation no longer holds, i.e. when there's sufficient kinetic energy that we can ignore the change due to the interaction. We'll say this is where $KE = \frac{Z_1 Z_2 e^2}{r}$, or $b_{\min} = \frac{Z_1 Z_2 e^2}{b_{\min}}$. For $b_{\max}$, we can pick the Debye length, at which point the particles feel a neutral environment.

$$L_D = \left(\frac{k_B T}{4\pi n_e e^2} \right)^{1/2} = b_{\max}. \tag{4.6}$$

Here, n_e is the free electron density.

We get

$$\langle \frac{\mathrm{d}}{\mathrm{d}t}(\Delta p_\perp)^2 \rangle = \frac{8\pi n_2 Z_1^2 Z_2^2 e^4}{v_1} \ln \Lambda \tag{4.7}$$

where $\ln \Lambda = \int_{b_{\min}}^{b_{\max}} \frac{\mathrm{d}b}{b}$. We call this the *Coulomb logarithm*, and it's approximately given by

$$\ln \Lambda = \ln \left[\frac{E}{k_B T} \frac{(kT)^{3/2}}{(4\pi n_e)^{1/2} Z_1 Z_2 e^2} \right] = 22.1 + \ln \left[(fracEkT) \left(\frac{T}{10^4 \mathrm{K}} \right)^{3/2} \left(\frac{n_e}{1 \mathrm{cm}^{-3}} \right)^{-1} \right]. \tag{4.8}$$

Reasonable numbers for this logarithm are around 20-30. This is likely to break down when the particles no longer form a fluid.

On what length scales can we treat a plasma as a fluid?

$$t_{\mathrm{defl}} = \frac{(m_1 v_1)^2}{\langle \frac{\mathrm{d}}{\mathrm{d}t}(\Delta p_\perp)^2 \rangle} = \frac{m_1^2 v_1^3}{8\pi n_2 Z_1^2 Z_2^2 e^4 \ln \Lambda}. \tag{4.9}$$

This gives us an effective mean free path,

$$\lambda_{\mathrm{mfp}} = v_1 t_{\mathrm{defl}} = \frac{m_1^2 v_1^4}{8\pi n_2 Z_1^2 Z_2^2 e^4 \ln \Lambda}. \tag{4.10}$$

As an example, consider electrons being deflected by either electrons or protons. Assume an initial velocity corresponding to a kinetic energy of $\frac{3}{2}k_B T$, i.e. set by the temperature of the gas.

$$\lambda_{\text{mfp}} = 5 \times 10^{12} \left(\frac{m_1}{m_e}\right)^2 \left(\frac{T}{10^4 \text{K}}\right)^2 \left(\frac{n_2}{0.1 \text{cm}^{-3}}\right)^{-1} \left(\frac{\ln \Lambda}{25}\right)^{-1} \text{cm}. \qquad (4.11)$$

The prefactor is about one third of an AU.

Many times, the ISM is not in local thermodynamic equilibrium (LTE). This is because

- We have low densities and therefore low collision rates.

- The radiation field is often not generated locally.

- Radiative de-excitation of energy levels can happen quickly compared to collisions; generally, $T_{\text{kin}} \neq T_{\text{exc}}$.

To look at this in more detail, let's ask about the timescale over which particles reach thermodynamic equilibrium. Consider a particle (particle 1) with velocity v_1 and kinetic energy $\frac{1}{2}mv_1^2$, in a fluid of particles with mass m_2. With each encounter, particle 1 gives some momentum $\Delta p_\perp$ to a field particle, and its energy decreases by $\frac{(\Delta p_\perp)^2}{2m_2}$.

The time required for encounters to completely deplete particle 1's excess energy E is

$$t_{\text{loss}} \equiv \frac{E}{\left\langle \left(\frac{\text{d}E}{\text{d}t}\right)_{\text{loss}} \right\rangle}. \qquad (4.12)$$

Here, $\left\langle \left(\frac{\text{d}E}{\text{d}t}\right)_{\text{loss}} \right\rangle$ is the average rate at which the particle gives KE to field particles, and we can calculate it from the transfer of momentum:

$$t_{\text{loss}} = \frac{m_1 v_1^2}{\left\langle \frac{\text{d}}{\text{d}t} (\Delta p_\perp)^2 / m_2 \right\rangle} = \frac{m_1 m_2 v_1^3}{8\pi n_2 Z_1^2 Z_2^2 e^4 \ln \Lambda}. \qquad (4.13)$$

For example, how long would it take for encounters to slow down fast electrons in a sea of protons? We can plug in numbers to this and get

$$t_{\text{loss}} = 0.4 \left(\frac{T_e}{10^4 \text{K}}\right)^{3/2} \left(\frac{n_p}{1 \text{cm}^{-3}}\right)^{-1} \left(\frac{\ln \Lambda}{25}\right)^{-1} \text{Myr}. \qquad (4.14)$$

So it takes about a million years. The electrons and protons exchange energy very slowly because of the mass difference between them: each electron is slowed down a lot by each interaction, but each proton isn't, so the electrons can thermalize quickly and the protons can't and they can't reach the same temperature. This is called a "two-temperature plasma", where we have particles at two different central velocities, each described by a Maxwellian distribution at that central velocity.

4.2 The law of mass action and principle of detailed balance

Consider a system with volume V and temperature T. This system has a number of possible energy levels E_i, starting with a lowest state at E_0. Each level has a degeneracy g_i (multiple states with the same energy level.) Our question is going to be: for a system at temperature T, what is the total number of energy states that are accessible to the system? This is provided by the *partition function*,

$$Z(T) = \sum_S e^{-E_s/kT}.$$

(4.15)

We get Z from considering translational partitioning and internal states of each individual particle,

$$Z(T) = Z_{\text{tran}}(T) \times Z_{\text{int}}(T).$$

(4.16)

We usually care about the partition function per unit volume for a particle with mass m_X:

$$f(T) = \frac{Z(T)}{V} = \left[\frac{(2\pi m_x k_B T)^{3/2}}{h^3} \right] \times \sum_i g_i e^{-E_i/kT}.$$

(4.17)

Suppose we have some process by which the particles are interacting (we won't be specific about what this is yet). We can work with the forward and backward rates due to some reaction $R_1 + R_2 + \cdots + R_M \leftrightarrow P_1 + P_2 + \cdots + P_N$; we'll simplify this to $A + B \leftrightarrow C$. Recall the reaction rate is

$$\frac{\text{reactions}}{\text{cm}^3} = k_{AB} n_A n_B.$$

(4.18)

The principle of detailed balance states that the forward and backward reactions must balance:

$$k_{AB} n_A n_B = k_C n_C \implies \frac{k_{AB}}{k_C} = \frac{n_C}{n_A n_B}.$$

(4.19)

Note that k_{AB} is a reaction rate per unit volume, but k_C is just a reaction rate. We also have the *law of mass action*,

$$\frac{n_C}{n_A n_B} = \frac{f(C)}{f(A)f(B)}.$$

(4.20)

Here, f is the partition function. Next time, we'll apply this to collision rates and see how it'll be useful.

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Lecture 5: Atomic and molecular structure

Lecturer: Nia Imara   *12 October*   *Aditya Sengupta*

Let's apply what we saw last lecture to collision rates. Suppose we have a species X which can be in two states l and u, which we denote $X(l)$ and $X(u)$. Collisions between X and Y cause collisional excitations or de-excitations between the states in X. Assuming Y doesn't change during the reaction, we have

$$X(l) + Y \leftrightarrow X(u) + Y. \tag{5.1}$$

When we apply the principle of detailed balance and the law of mass action, we get

$$\frac{k_{ul}}{k_{lu}} = \frac{n_{X_l} n_Y}{n_{X_u} n_Y} = \frac{n_{X_l}}{n_{X_u}} = \frac{f(X_l)}{f(X_u)} = \frac{z_{\text{int}}(X(l), T)}{z_{\text{int}}(X(u), T)} \tag{5.2}$$

where the translational parts of the partition functions cancel because they have the same temperature.

Suppose the upper and lower states have energies E_u, E_l and degeneracies g_u, g_l. Then

$$z_{\text{int}}(X(l), T) = g_l \exp(-E_l/kT) \tag{5.3}$$

and respectively u. Therefore

$$\frac{k_{ul}}{k_{lu}} = \frac{g_l}{g_u} \exp\left(\frac{E_{ul}}{kT}\right) \tag{5.4}$$

where $E_{ul} = E_u - E_l$.

We have related the rates of collisional excitation and de-excitation for a given species solely in terms of T, the degeneracies of the levels, and the energy difference between them.

This is signfiicant because we can calculate the coefficient rate for various processes, including those involving the absorption and emissions of photons. This will let us calculate relative strengths of different atomic and molecular species in a given environment, which we'll later use in turn to form relationships between the Einstein coefficients, which describe the probability that particles absorb or emit radiation. We'll look at systems with multiple energy levels that are relevant to the ISM, like the 21cm neutral hydrogen line and the CO line.

To fully understand the physics, we'll need to understand:

- Given some atom, ion, or molecule, what sets the spacing between energy levels?

- How frequently do transitions between the various levels occur?

n	l	m_l	subshell label	number of orbitals	number of possible states
1	0	0	1s	1	2
2	0	0	2s	1	2
	1	-1, 0, 1	2p	3	6
3	0	0	3s	1	2
	1	-1, 0, 1	3p	3	6
	2	-2, -1, 0, 1, 2	3d	5	10
4	0	0	4s	1	2
	-1	-1, 0, 1	4p	3	6
	2	-2, -1, 0, 1, 2	4d	5	10
	3	-3, -2, -1, 0, 1, 2, 3	4f	7	14

Table 5.1: The allowed quantum states for $n = 1, 2, 3, 4$.

Energy levels of atoms depend on where the electrons are and their angular momentum. The state of a molecule is described by the quantum numbers:

- n is the principal quantum number. It describes the main energy level ($n \geq 1$).

- l is the orbital angular momentum in units of $\hbar$ ($0 \leq l < n$); it describes the shape of the orbital.

- m_l is the magnetic quantum number, the component of l projected on the z axis ($-l \leq m_l \leq l$); it describes the orientation of the orbital.

- m_s is the spin angular momentum, the intrinsic spin of electrons within each orbital ($m_s = \pm\frac{1}{2}$ in units of $\hbar$).

In the absence of a magnetic field, only the first two states affect the electron energy. The spin states are degenerate (have the same energy).

We'll refer to n as the "shell". The orbitals with $l = 0, 1, 2, 3$ are designated by the letters *s, p, d, f*, and the combination of n, l is referred to as a "subshell".

Subshells are filled in order of increasing $n + l$, and then in order of increasing n; this is how you get the pattern of 1s, 2s, 2p, 3s, 3p, 4s, ...

In an unfilled subshell, there are multiple possibilities for distributing electrons, which leads to a different overall angular momentum. We'll say L is the sum of angular momenta l_i, S is the sum of spin angular momenta s_i, and $J = L + S$ is the total angular momentum. We have $2L + 1$ degenerate levels for m_l and $2S + 1$ degenerate levels for m_s. So each (L, S) has $(2L + 1)(2S + 1)$ possible states within it.

This matters because different combinations of L and S have different angles. $L - S$ coupling describes how the total spin S interacts with the total angular momentum L ("spin-orbit coupling"). A larger spin means there are more individual spins aligned in the same direction, and electrons are further apart on average. So a larger spin usually has lower energy.

In the *L-S coupling approximation*, we can characterize this configuration as a vector sum of the orbital angular momentum $L\hbar$ and of the individual spin angular momenta $S\hbar$. A particular value of an (L, S) combination is called a *spectroscopic term*. This approximation is only good for light atoms, because after that we have relativistic corrections.

We denote spectroscopic terms by

$$^{2S+1}\mathcal{L}_J^p$$

where S is the spin, p is the parity $\sum_i l_i$, and J is the total angular momentum. Here, $\mathcal{L}$ is replaced by the orbital angular momentum, starting with S, P, D, F.

For example, for the ground state of HI, we have an electronic configuration of $1s^1$. $l_1 = 0$, so $L = 0$, and $s_1 = \frac{1}{2}$ so $S = \frac{1}{2}$, so we have $^2S_{1/2}$. Finally, $p = 0$, so we don't write anything.

Similarly, for HeI, we have $1s^2$. We have $l_1 = 0, l_2 = 0$ and so $L = 0$, and $s_1 = \frac{1}{2}, s_2 = -\frac{1}{2}$, so $S = 0$. Therefore we have $^1S_0$.

Diffuse Matter in Space	**Fall 2023**

Lecture 6: Molecular structure and radiative transfer

Lecturer: Nia Imara   *17 October*   *Aditya Sengupta*

We want to understand the energy-level structure of atoms and molecules, and understand the nomenclature referring to those levels. In doing this, we'll understand the origin of some important transitions in the ISM, like the 21cm line, hyperfine transitions, and CO emission.

Last time, we saw that spectroscopic terms are a way of understanding what's going on when there's multiple ways to fill up an electron configuration:

$$^{2\mathbf{S}+1}\mathcal{L}_{\mathbf{J}}^{p}$$

where the $\mathcal{L}$ describes orbital angular momentum, p describes parity, $\mathbf{J}$ describes total angular momentum, and $\mathbf{S}$ describes spin.

Last time, we were looking at the ground state of singly ionized HeII, $1s^1$. This has a spectroscopic term $^2S_{1/2}$, the same as the ground state of HI.

Let's derive the spectroscopic term for the ground state of C, $1s^2\ 2s^2\ 2p^2$. The first four electrons are in full shells, so their configuration is fixed. Since they're filling into 2p, we have $l = 1$, so $m_l \in \{-1, 0, 1\}$. Further, we have spin-up and spin-down states for each ($m_s = \pm\frac{1}{2}$), so we have six possible states for two indistinguishable particles and they can't share the same one. This means we have $\binom{6}{2} = 15$ possible configurations.

We can enumerate these 15 configurations and add up the resulting total m_L and m_S from the two electrons. The configurations are given in 6.1.

Some of these show up more than once, but under the L-S approximation, if these numbers are the same we consider the states to be interchangeable. But all the different states still do matter for Since $m_{\mathbf{L}}$ maxes out at 2, we must have a state with $\mathbf{L} = 2$. Further, we see only $(2, 0)$, so $\mathbf{S} = 0$ in this case. There are $(2L + 1)(2S + 1) = 5$ possible states for $L = 2, S = 0$.

Next, we have unaccounted-for states like $(1, 1)$, and since these aren't covered under the $\mathbf{L} = 2$ case, we group these under $\mathbf{L} = 1$. Then $\mathbf{S} = 1$ because we see $(1, 1)$, $(1, -1)$ states, etc. Finally, we also see an $\mathbf{L} = 0, \mathbf{S} = 0$ state.

We can now write down the spectroscopic terms corresponding to these: we see $^1D_2, ^3P_{0,1,2}, ^1S_0$. Note that when $L > 0$ and $S > 0$, their vector sum can be formed in multiple ways, so J goes from $|L - S|$ to $|L + S|$.

Which of these substates has the lowest or highest energy? The answer is given by Hund's rules:

1. The largest value of $\mathbf{S}$ is the lowest energy state. In our case, this means the ^3P states are the lowest energy.

2. For states with the same S, the largest L has the lowest energy state. This means ^1D is lower-energy than ^1S.

3. If the shell is less than half full, the lowest J is the lowest energy state; if it is more than half full, the highest J has the highest energy.

Electron 1		Electron 2	
m_l	m_s	m_l	m_s
1	½	0	½
1	½	-1	½
1	½	1	-½
1	½	0	-½
1	½	-1	-½
0	½	-1	½
0	½	1	-½
0	½	0	-½
0	½	-1	-½
-1	½	1	-½
-1	½	0	-½
-1	½	-1	-½
1	-½	0	-½
1	-½	-1	-½
0	-½	-1	-½

Figure 6.1: m_l and m_s configurations for the ground state of carbon.

When $L, S > 0$, there is more than one way to add $\vec{L}$ and $\vec{S}$ to get the total angular momentum $\vec{J} = \vec{L} + \vec{S}$. For a given value of L, S, the magnitude of $\vec{J}$ ranges from $|L - S|$ to $|L + S|$. Each configuration will have a different value $\vec{L} \cdot \vec{S}$ and will differ in energy due to spin-orbit coupling. This causes energy changes of the order 10^{-2} eV. This is called *fine structure*.

To understand fine structure, we'll look at an electrostatic picture of a nucleus-electron system. We have a nucleus with charge Ze and an electron at a distance r. From the electron's point of view, the electron is a moving charge, and this induces a magnetic field on the electron. The interaction of the electron's magnetic moment with this magnetic field is called *spin-orbit coupling*, and this is slightly different based on the electron's angular momentum.

If the nucleus also has a magnetic moment, each fine structure level may further split due to interactions between the B field of the nucleus and of the electron. This is the *hyperfine structure*. These splittings are of order 10^{-6} eV, corresponding to radio emission. The quantum numbers for hyperfine splitting are J, I, F, corresponding to something we don't really need to remember.

The hydrogen atom is the most important case of hyperfine splitting. The proton on a hydrogen atom has a spin of $\frac{1}{2}$, so depending on whether this is aligned to the electron spin ($F = 1$) or not ($F = 0$), we have a difference in energy levels of about 6.7×10^{-6} eV. This corresponds to a photon with $\lambda \approx 21$cm.

We've now worked out the basic structure of atoms, and would like to say something about the rate of radiative transitions between them. Transitions have to obey certain "selection rules", which are:

1. The parity has to change.

2. $\Delta L = 0, \pm 1$

3. $\Delta J = 0, \pm 1$, but $J = 0 \rightarrow 0$ is forbidden

4. Only one single electron wavefunction **nl** changes, with $\Delta l = \pm 1$.

5. $\Delta S = 0$: spin does not change.

We say that

- **allowed transitions** satisfy all rules;

- **semi-forbidden transitions** satisfy all rules except the last one; and

- **forbidden transitions** violate at least one rule other than the last one.

Semi-forbidden and forbidden transitions can actually happen, but they're highly improbable.

An example of an allowed transition and how we write it down is NII 1084.0 Å^{3}P$_0 - ^3$D$_1$○. We can check if this satisfies all the selection rules:

- The parity changes (check what this means)

- $\Delta L = -1$, because we're going from 2 to 1.

- $\Delta J = -1$, because we're going from 1 to 0.

- We have an electron going from 3s to 2p and nothing else changing, so we have $l = 1$ going to $l = 0$ and $\Delta l = -1$.

- The spin does not change.

For allowed transitions, we can write down an Einstein coefficient, and the inverse of that is the lifetime. In this case, the transition has a lifetime of 4.6 ns. Allowed transitions tend to happen very fast.

Consider the semi-forbidden transition N II] 2143.4 Å$^5 textS_2 \circ - {}^3P_2$.

- The parity changes from odd to even.

- $\Delta L = -1$

- $\Delta J = 0$, but we don't have $J = 0 \to 0$.

- The electron wavefunction goes from $l = 1$ to $l = 0$ and $\Delta l = -1$.

- The spin changes.

This works over a timescale of milliseconds, about six orders of magnitude slower.

Finally, let's look at the forbidden transition [N II] 6549.9 Å$^3P_1 - {}^1D_2$.

- The parity does not change (so this rule is violated).

- $\Delta L = -1$

- $\Delta J = 1$.

- The electron wavefunction does not change, $\Delta l = 0$.

- $\Delta S = 0$.

The lifetime of this transition is about 20 minutes.

Even forbidden transitions can be incredibly important in the ISM.

The C+ fine structure transition at 158μm is the most important coolant of the warm ISM. Most carbon in the ISM is in the form of C+ ions. Since carbon has a lower ionization energy than H, it'll be in the form of C+ in the neutral surface layers of FUV-illuminated gas clouds. It's possible to study this with ALMA, and this helps us determine whether C II outflows can suppress star formation.

In diatomic molecules, we have rotational and vibrational motion that can cause transitions. We can also have transitions due to changes in electron energy levels. By the Born-Oppenheimer approximation, as long as rotation/vibration of nuclei is slow compared to typical electron speeds, the electron energies are unaffected so we can treat them separately.

Let's consider rotation first. We have two masses m_1, m_2 with a reduced mass $m_r = \frac{m_1 m_2}{m_1 + m_2}$ and a separation r_n. These have a moment of inertia $I = m_r r_n^2$. These have a rotational energy of

$$E_{\text{rot}} = \frac{J(J+1)\hbar^2}{2m_r r_n^2} = J(J+1)B_v \tag{6.1}$$

where J is the rotational quantum number. Here, we say $B_v \equiv \frac{\hbar^2}{2m_r r_n^2}$ is the rotation constant, and v represents the vibrational state.

The rotation constant can be given in terms of scaling factors as

$$B_v = 24 \left(\frac{m_r}{m_H} \right)^{-1} \left(\frac{r_n}{1\text{Å}} \right)^{-2} \text{K} \cdot k. \tag{6.2}$$

For example, consider the first excited state ($J = 1 \to 0$) for diatomic hydrogen and CO. H_2 has a reduced mass of $m_H/2$ and $E/k = 170$ K. CO has $m_r = 6.9 m_H$ and $E/k = 5.5$K. Because H_2 is such a light molecule, its first excited state requires a lot of energy. But since the dense ISM where molecules form is usually cold (about 10K), almost no molecules exist in this state.

Lecture 7: Einstein coefficients and line profiles

Lecturer: Nia Imara *19 October* *Aditya Sengupta*

Last time, we were looking at the energy levels of diatomic molecules. As a function of internuclear separation, there's a minimum carved out by the balance between electronic and rotational transitions.

Vibrational potential energy can be approximated as a harmonic oscillator around this minimum. There's a fundamental frequency of the oscillator $\omega = \left(\frac{k}{m_r}\right)^{1/2}$, and this defines vibrational energy levels according to $E_{\text{vib}} = \hbar\omega(n + \frac{1}{2})$. This lets us define a total energy based on quantum numbers (v, J):

$$E_q(v, J) = V_q(r_0) + \hbar\omega\left(v + \frac{1}{2}\right) + B_v J(J + 1). \tag{7.1}$$

Generally, $\hbar\omega \gg B_v$, so rotational energy levels for a given v are much more closely spaced than for vibrational ones.

Heteronuclear molecules (two different nuclei) have permanent dipole moments, while homonuclear molecules (two of the same nuclei) don't have permanent dipole moments.

With a rotating dipole, the Einstein coefficient for electric dipole transitions is

$$A_{J,J-1} = \frac{128}{3\hbar}\left(\frac{B_v}{hc}\right)^3 \mu^2 \frac{J^4}{J + 1/2} \tag{7.2}$$

For CO $J = 1$, this comes out to about 5 months.

H_2 is the most common molecule in the ISM. The protons are identical fermions, so they have to obey the Pauli exclusion principle. We can have a total nuclear spin of $l = 1$ or $l = 0$, and the Pauli exclusion principle fixes J in both of these cases. If $l = 0$, we have J even and we have para-H_2; if $l = 1$, we have J odd and we have ortho-H_2. Conversions between the two states only happen via collisions, which are rare in the ISM. So these species are effectively decoupled.

There are essentially no radiative transitions from H_2, so it is unobservable in emission. This is because it's diatomic and homonuclear, so it has no permanent dipole moment and no corresponding rotational transitions. The energy level spacings vary as $m_r^{1/2}$, so they're too close together to easily detect transitions.

Einstein was the first to describe the relationship between emission and absorption at a microscopic level. In a two-level system, there's three processes: spontaneous emission, absorption, and stimulated emission.

1. Spontaneous emission occurs when the system is in level u and drops to level l by emitting a photon.

2. Absorption occurs when the system transitions from level l to u by absorbing a photon with $E = h\nu$. The transition probability per unit time is proportional to the mean intensity of photons at frequency ν. The relative probability that a photon of frequency ν will be absorbed is described by a line profile function ϕ_ν.

3. Stimulated emission occurs when a downward transition is induced by an incoming photon at a frequency identical to an energy level distance.

In thermodynamic equilibrium, we have a rate relation,

$$n_l B_{lu} \bar{J} = n_u A_{ul} + n_u B_{ul} \bar{J}. \tag{7.3}$$

Solving for $\bar{J}$, we get

$$\bar{J} = \frac{A_{ul}/B_{ul}}{(n_l/n_u)(B_{lu}/B_{ul}) - 1}. \tag{7.4}$$

Recall that in LTE, we have

$$\frac{n_l}{n_u} = \frac{g_l}{g_u} \exp\left(-\frac{h\nu}{kT}\right). \tag{7.5}$$

In LTE, we also know that $J_\nu = B_\nu$. Also, if we approximate ϕ_ν as a delta function, we can say $\bar{J} = B_\nu$. So combining these things, we can relate the Einstein coefficients to the temperature and frequency:

$$\frac{A_{ul}/B_{ul}}{(g_l B_{lu}/g_u B_{ul}) \exp(h\nu/kT) - 1} = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT) - 1}. \tag{7.6}$$

Mathematically, for this expression to hold for all temperatures, we need the prefactor on the $\exp(h\nu/kT)$ and the prefactor overall to be equal, so this gives us

$$B_{lu} = \frac{g_u}{g_l} B_{ul} \tag{7.7}$$

$$B_{ul} = \frac{c^2}{2h\nu^3} A_{ul}. \tag{7.8}$$

This means if we measure A_{ul} in the laboratory and know the degeneracy of the population we care about, we can derive the B coefficients. Note that temperature isn't involved, so these have to hold whether or not the particles are in thermodynamic equilibrium. Optical properties depend on the Einstein coefficients.

Note that we're using the Einstein B coefficient conventions of Rybicki and Lightman, relative to the radiation intensity, while Draine defines them relative to the radiation energy density. These are off by a factor of $\frac{c}{4\pi}$.

It's often convenient to recast the absorption and stimulated emission processes in terms of a cross section. Let $\sigma_{lu}(\nu)$ represent the $l \to u$ transition (absorption) and $\sigma_{ul}(\nu)$ the $u \to l$ transition (stimulated emission). We don't need to factor in spontaneous emission because that happens independently of incoming radiation.

Using a formalism analogous to what we did for collisions, we can write down

$$\sigma_{lu}(\nu) = \frac{g_u}{g_l} \frac{c^2}{8\pi\nu^2} A_{ul}\phi_n u \tag{7.9}$$

$$\sigma_{ul}(\nu) = \frac{g_l}{g_u}\sigma_{lu}(\nu). \tag{7.10}$$

At this point, we could ask: why isn't $\sigma_{lu}(\nu)$ an infinitely sharp delta function? It seems like this would involve a photon whose energy isn't the energy difference between the two levels being absorbed. Some of this is quantum uncertainty in the energy, but even without that, for particles at a finite temperature, there's a range of velocities and due to the Doppler effect there's many allowed velocities that provide the correct energy.

A number of physical mechanisms can broaden the line profile:

- The natural lifetimes of excited states

- Thermal motions due to the Doppler effect

- Collisions

- Turbulent bulk motions

We'll focus on natural broadening due to the uncertainty principle ($\Delta E \Delta t \geq \hbar$, where Δt is the lifetime of the state) and Doppler broadening due to the spread in velocity of particles in the gas. Natural broadening has a width in frequency space of $\Delta\nu = \frac{1}{2\pi\Delta t}$. More precisely, we have a Lorentz profile:

$$\phi_\nu \approx \frac{4\gamma_{ul}}{16\pi^2(\nu - \nu_{ul})^2 + \gamma_{ul}^2}. \tag{7.11}$$

What is γ_{ul}? It's the sum of the Einstein A coefficients in both layers.

$$\gamma_{ul} = \sum_{j<u} A_{uj} + \sum_{j<l} A_{lj}. \tag{7.12}$$

It's the sum of all the relevant lifetimes ($\sim 1/A$) for the energy levels you are transitioning between.

Typical line widths for allowed UV and optical transitions are on the order of 10 m/s, while for X-ray transitions they can reach 10 km/s. The most prominent example is Lyman-α, with $(\Delta\nu)_{\text{FWHM}} \sim 0.0121$ km/s.

Usually the Doppler width is much larger than the natural width because we have thermal velocities much greater than 10 m/s. The expression for Doppler broadening is a Gaussian:

$$\phi_\nu = \frac{1}{\sqrt{2\pi\sigma_v^2}} \exp\left(-\frac{(\nu - \nu_0)^2}{2\sigma_v^2}\right). \tag{7.13}$$

In reality, both Doppler and natural broadening happen at the same time, so the true line profile is a convolution of the two:

$$\phi_\nu = \frac{1}{\sqrt{2\pi\sigma_v^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{v^2}{2\sigma_v^2}\right) \frac{4\gamma_{ul}}{16\pi^2(\nu - (1 - v/c)\nu_{ul})^2 + \gamma_{ul}^2} \, \mathrm{d}v. \tag{7.14}$$

This is the *Voigt profile*.

(Radiation field definitions)

We have $I_\nu = B_\nu$ in LTE, and we have a brightness temperature T_B such that $B_\nu(T_B) = I_\nu$:

$$T_B(\nu) = \frac{h\nu}{\ln[1 + (2h\nu^3/c^2 I_\nu)]}. \tag{7.15}$$

We also have the *antenna temperature* T_A an approximate form of T_B that's linear with I_ν:

$$T_A(\nu) \equiv \frac{c^2}{2k v^2} I_\nu. \tag{7.16}$$

The excitation temperature of a level u relative to level l is defined by the Boltzmann law:

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} \exp\left(-\frac{E_{ul}}{kT_{exc}}\right). \tag{7.17}$$

Radiative transfer solution.

At a specific frequency, the rate of spontaneous decays is $n_u A_{ul} \phi_\nu$. So the emissivity is

$$j_\nu = \frac{1}{4\pi} n_u A_{ul} h\nu \phi_n u. \tag{7.18}$$

For attenuation, we look at absorption minus stimulated emission,

$$\kappa_n u = n_l \frac{h\nu}{4\pi} B_{lu} \left(1 - \frac{g_l}{g_u} \frac{n_u}{n_l}\right) \phi_\nu. \tag{7.19}$$

We can rewrite this in terms of brightness temperature, plug back into the radiative transfer equation, change variables so that we're integrating over optical depth, and solve.

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Lecture 8: Radiative transfer in physical contexts

Lecturer: Nia Imara   *24 October*   *Aditya Sengupta*

Last time, we were describing the probability of absorption and emission as described by the Einstein coefficients.

In local thermodynamic equilibrium, we have

$$n_l B_{lu} \bar{J} = n_u A_{ul} + n_u B_{ul} \bar{J}. \tag{8.1}$$

Let $\bar{J} = B_\nu$. Recall that the ratio of n_l and n_u is given by the BOltzmann distribution. Then

$$B_{lu} = \frac{g_u}{g_l} B_{ul} \tag{8.2}$$

$$B_{ul} = \frac{c^2}{2h\nu^3} A_{ul}. \tag{8.3}$$

It's often convenient to recast the Einstein coefficients in terms of cross-sections. We can show that

$$\text{absorption: } \sigma_{lu}(\nu) = \frac{g_u}{g_l} \frac{c^2}{8\pi\nu^2} A_{ul} \phi_\nu \tag{8.4}$$

$$\text{stimulated emission: } \sigma_{ul}(\nu) = \frac{g_l}{g_u} \sigma_{lu}(\nu) \tag{8.5}$$

where ϕ_ν describes a line profile, and $\int \phi_\nu \mathrm{d}\nu = 1$. The profiles are set by various physical *broadening* processes: natural broadening, the extent of which is set by the Einstein A coefficient, and Doppler broadening.

Last time, we also covered the radiative transfer equation.

$$\mathrm{d}I_\nu = -I_\nu \kappa_\nu \mathrm{d}s + j_\nu \mathrm{d}s. \tag{8.6}$$

We can describe a source in terms of its emission j_ν. On top of this, we use the opacity

$$\kappa_\nu = \frac{h\nu}{4\pi} n_l B_{lu} \left(1 - \frac{g_l}{g_u} \frac{n_u}{n_l}\right) \phi_\nu = \frac{h\nu}{4\pi} n_l B_{lu} \left(1 - e^{-E_{ul}/kT_{\text{exc}}}\right) \phi_\nu. \tag{8.7}$$

We can solve this to get

$$I_\nu(\tau_\nu) = I_\nu(0) e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau')} S_\nu \mathrm{d}\tau'. \tag{8.8}$$

Here, we're using $S_\nu = j_\nu/\kappa_\nu$ to represent the source function.

As a first example, consider an infinite, uniform slab of matter in LTE at temperature T. The energy levels must have $T_{\text{exc}} = T$. The radiation field must be equal to the Planck function, $I_\nu = B_\nu(T)$. It follows that

$$\mathrm{d}I_\nu = -B_\nu \mathrm{d}\tau_\nu + S_\nu \mathrm{d}\tau_\nu = 0. \tag{8.9}$$

Here, we can take $\mathrm{d}I_\nu = 0$ because the slab is infinite. Therefore the source function is $S_\nu = \frac{j_\nu}{\kappa_\nu} = B_\nu(T)$. This result is known as Kirchhoff's law. Since S_ν depends only on fundamental properties of the matter, this condition must hold in general, not just in equilibrium, if we replace $T \to T_{\text{exc}}$. Without loss of generality, we can substitute this into the formal solution to the transfer equation,

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau')} B_\nu(T_{\text{exc}})\mathrm{d}\tau'. \tag{8.10}$$

If we consider a constant temperature, this simplifies to

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + B_\nu(T_{\text{exc}})(1 - e^{-\tau_\nu}). \tag{8.11}$$

When $\tau_\nu \ll 1$, the radiation is relatively unchanged; when $\tau_\nu \gg 1$, the radiation becomes thermalized.

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Lecture 9: HI 21cm emission and absorption

Lecturer: Nia Imara	*26 October*	*Aditya Sengupta*

Reviewing part c of the practice problem from last time: we're given a rate A that we can convert to a number of photons emitted per unit area NA. Each of these photons carries energy $E = h\nu = 7.86 \times 10^{-3}$ eV. So the rate of energy emission is $F = NAE$.

The spin-flip transition of neutral hydrogen, due to hyperfine splitting, is one of the simplest transitions and one of the most important for looking at the ISM. This line occurs because in the ground state of neutral hydrogen, the state with parallel electron and nuclear spins has a different energy from the one with antiparallel spins. The energy difference is 5.87×10^{-6} eV, which corresponds to 21cm emission.

The excitation temperature T_{spin} depends on the region. Under normal circumstances, we must have $T_{\mathrm{spin}} > T_{\mathrm{CMB}} = 2.72$K. Since $T_{\mathrm{spin}} \gg T_{\mathrm{ul}}$, the Boltzmann factor $\exp(-E_{\mathrm{ul}}/kT_{\mathrm{spin}}) \approx 1$, and

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} \exp\left(-\frac{E_{\mathrm{ul}}}{kT_{\mathrm{spin}}}\right) \approx 3. \tag{9.1}$$

The levels are approximately populated by their degeneracy because the exponential factor is about 1. Therefore at any given time we expect $3/4$ of the atoms to be in the upper hyperfine state and $1/4$ to be in the lower state.

We can compute the emissivity and attenuation:

$$j_\nu = \frac{3}{16\pi} h\nu_{ul} n_H A_{ul} \phi_\nu \tag{9.2}$$

$$\kappa_\nu = \frac{3}{32\pi} A_{ul} \frac{hc\lambda_{ul}}{kT_{\mathrm{spin}}} n_H \phi_\nu. \tag{9.3}$$

What opacity does this give us? Consider a slab of hydrogen of length L:

$$\tau_\nu = \kappa_\nu L = \frac{3}{32\pi} A_{ul} \frac{hc\lambda_{ul}}{kT_{\mathrm{spin}}} N_H \phi_\nu \tag{9.4}$$

where $N_H = n_H L$ is the column density of H atoms.

If we consider a Gaussian line profile, we get

$$\tau_\nu = 2.19 \left(\frac{N_H}{10^{21}\mathrm{cm}^{-2}}\right) \left(\frac{T_{\mathrm{spin}}}{100\mathrm{K}}\right)^{-1} \left(\frac{\sigma_v}{\mathrm{km/s}}\right)^{-1} \exp\left(-\frac{v^2}{2\sigma_v^2}\right). \tag{9.5}$$

If all these coefficients were order unity, we'd have optically thick HI emission everywhere. But in reality there's often much higher spin temperatures.

Observations of optically thin 21cm emission is the basis for all estimates of the atomic gas masses of galaxies. For an optically thin line of sight, we can ignore absorption:

$$\int dI_\nu = \int j_\nu ds \implies I_\nu = I_\nu(0) + \frac{3}{16\pi} A_{ul} h \nu_{ul} \phi_\nu N_H \tag{9.6}$$

where $N_H = \int n_H ds$. If we integrate over frequency, we have

$$N_H = \frac{16\pi}{3 A_{ul} h \nu_{ul}} \int [I_\nu - I_\nu(0)] d\nu \tag{9.7}$$

and we can translate this to antenna temperature $T_A = \frac{c^2}{2k\nu^2} I_\nu$, and relate velocity to frequency via the Doppler shift, $\nu = \nu_{ul}(1 - \frac{v}{c})$. This giveds us the velocity-integrated antenna temperature,

$$\int [T_A - T_A(0)] dv = \int \frac{c^2}{2k\nu^2} [I_\nu - I_\nu(0)] \frac{c}{\nu} d\nu = \frac{3}{32\pi} \frac{hc\lambda_{ul}^2}{k} A_{ul} N_H. \tag{9.8}$$

This gives us

$$\int [T_A - T_A(0)] dv = 54.89 \text{K km/s} \left(\frac{N_H}{10^{20} \text{cm}^{-2}} \right). \tag{9.9}$$

If we resolve the object we're looking at, this gives us the column density. If the emitting object is unresolved, we can't directly measure the intensity (T_A) but we can measure the total flux if we know the distance.

$$F = \int I_\nu d\nu \frac{dA}{D^2}. \tag{9.10}$$

For simplicity, we drop the background term $I(0)$, and we get a total hydrogen mass $M_H = m_H \int N_H dA$, so

$$F = \frac{3 A_{ul} h \nu_{ul}}{16\pi D^2} \frac{M_H}{m_H} \tag{9.11}$$

which in power-law form gives us

$$M_H = 4.95 \times 10^7 \text{M}_\odot \left(\frac{D}{\text{Mpc}} \right)^2 \left(\frac{F}{\text{Jy MHz}} \right). \tag{9.12}$$

Doing radiative transfer through this, we get

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + B_\nu(T_{\text{spin}})(1 - e^{-\tau_\nu}). \tag{9.13}$$

Since $kT_{\text{spin}} \gg h\nu$, we can say $B_\nu(T_{\text{spin}}) \approx \frac{2k\nu^2}{c^2}T_{\text{spin}}$ and

$$T_A(\tau_\nu) = T_A(0)e^{-\tau_\nu} + T_{\text{spin}}(1 - e^{-\tau_\nu}). \tag{9.14}$$

If we take a measurement on-source and off-source for, say, a quasar, we have

$$\tau_\nu = \ln\left(\frac{T_{QSO} - T_{sky}}{T_A^{on} - T_A^{off}}\right) \tag{9.15}$$

and

$$T_{spin} = \frac{T_A^{off}T_{QSO} - T_A^{on}T_{sky}}{(T_{QSO} - T_{sky}) - (T_A^{on} - T_A^{off})}. \tag{9.16}$$

HI self-absorption and cold regions, tbd off the slides. HISA sometimes follows the distribution of CO emission.

Lecture 10: Absorption lines

Lecturer: Nia Imara *2 November* *Aditya Sengupta*

Suppose we observe a bright continuum point source. Since most of the ISM is cold, we have $n_u/n_l \ll 1$, and so the more significant part of the radiative transfer equation is the original part of the source:

$$F_\nu = F_\nu(0) \exp(-\tau_\nu). \tag{10.1}$$

We can measure the amount of flux that's "missing" over a frequency range centered on some ν_0. If we plot $F_\nu/F_\nu(0)$, we get a dip to almost 0 at ν_0 and we see 1 further away.

It's useful to define an integral over the line called the *equivalent width*.

$$W = \int \left(1 - \frac{F_\nu}{F_\nu(0)}\right)\frac{\mathrm{d}\nu}{\nu_0} = \int (1 - \exp(-\tau_\nu))\frac{d d\nu}{\nu_0}. \tag{10.2}$$

W is a dimensionless number characterizing the fraction of light that has been absorbed. Note that sometimes you'll see $W_\lambda = W\lambda_0$.

If we measure the equivalent width, we get the column density of the absorbers. The attenuation coefficient for line absorption gives us an optical depth,

$$\tau_\nu = \frac{h\nu}{4\pi}N_l B_{lu}\left(1 - \frac{g_l}{g_u}\frac{n_u}{n_l}\right)\phi_\nu. \tag{10.3}$$

Here, $N_l = \int n_l \mathrm{d}s$.

Instead of the Einstein coefficient, we often write this relation in terms of the oscillator strength

$$f_{lu} = \frac{m_e c}{\pi e^2}\int \sigma_{lu}(\nu)\mathrm{d}\nu. \tag{10.4}$$

This is a fraction explaining the contribution of quantum mechanics to the probability that a particular atom absorbs an approaching photon. Each possible transition has a unique oscillator strength. This is related to the Einstein A according to

$$A_{ul} = \frac{8\pi^2 e^2 \nu_{ul}^2}{m_e c^3}\frac{g_l}{g_u}f_{lu}. \tag{10.5}$$

With these definitions, we have

$$\tau_\nu = \frac{\pi e^2}{m_e c^2} f_{lu} N_l \left(1 - \frac{g_l}{g_u}\frac{n_u}{n_l}\right)\phi_\nu \tag{10.6}$$

and in cold interstellar gas, we have n_u/n_l negligible, so

$$\tau_\nu = \frac{\pi e^2}{m_e c^2} f_{lu} N_l \phi_\nu. \tag{10.7}$$

The line profile is generally a Voigt profile, but at the line core we'll say it's a Gaussian. Substituting this in and considering a Doppler broadening parameter $b = \sqrt{2}\sigma_\nu$, we get (for the optical depth at the line center)

$$\tau_0 = \sqrt{\pi}\frac{e^2}{m_e c^2}\frac{f_{lu}\lambda_{ul}N_l}{b}. \tag{10.8}$$

In power-law form this is

$$\tau_0 = 0.758 \frac{N_l}{10^{13}\text{cm}^{-2}}\frac{f_{lu}}{0.4164}\frac{\lambda_{ul}}{1215.7\text{Å}}\frac{10\text{km/s}}{b}.$$

The optical depth in the Gaussian part of the line is

$$\tau_\nu = \tau_0 \exp\left(-u^2/b^2\right) \tag{10.9}$$

where $u = c(\nu_0 - \nu)/\nu_0$ is the velocity shift required to produce a frequency shift of ν.

Since we won't necessarily resolve the line, we're just measuring the integral, so we consider the *equivalent width*.

For $\tau_\nu \ll 1$ we have $W \propto N$, and for $\tau_\nu \sim 10 - 1000$, we can find that $W \propto b\sqrt{\ln(N/b)}$. There's only marginal increases in the equivalent width with increasing column density. At a certain point, our $F_\nu/F_\nu(0)$ curve flattens out and we have *saturated lines*. For $\tau_n u \geq 10^4$, $W \propto \sqrt{N}$. We see wings develop at frequencies away from ν_0. There's math to find all of this.

Wings begin to dominate at $N_l \sim 10^{19}\text{cm}^{-2}$ or $\tau_0 \approx 10^5$ for Lyman-alpha absorption.

If we can't directly measure the line shape and we only have the EW, we don't know b or τ_0, we don't know where we are on the curve of growth, and so we can't reliably measure the column density. To fix this, we consider *doublet ratios*, where we take the ratio of two equivalent widths.

The ratio of two equivalent widths (e.g. two lines in a doublet) can be a sensitive indicator of location on the curve of growth. WLOG let's say that $f_{lu2}\lambda_{lu2} > f_{lu1}\lambda_{lu1}$. We have three regimes:

$$\frac{W_2}{W_1} = \begin{cases} \frac{f_{lu_2}\lambda_{lu_2}}{f_{lu_1}\lambda_{lu_1}} & \text{optically thin} \\ \left[1 + \frac{\ln\left(f_{lu_2}\lambda_{lu_2}/f_{lu_1}\lambda_{lu_1}\right)}{\ln(\tau_{0,1}/\ln 2)}\right]^{1/2} & \text{saturated} \\ \frac{\lambda_{lu_2}}{\lambda_{lu_1}}\sqrt{\frac{f_{lu_2}\gamma_{lu_2}}{f_{lu_1}\gamma_{lu_1}}} & \text{damped.} \end{cases} \tag{10.10}$$

In each regime, the line ratio takes on a value determined (almost) solely by atomic constants, so by measuring the line ratio, we can learn what part of the curve of growth we're on, and which formula we should use to compute the column N_l.

Diffuse Matter in Space **Fall 2023**

Lecture 11: Optical properties of dust

Lecturer: Nia Imara *7 November* *Aditya Sengupta*

Dust causes starlight extinction at short wavelengths, and we can map this out over the sky. We can also observe dust in emission at longer wavelengths.

The polarization of light refers to the orientation of the waves. A light wave vibrating in more than one plane is unpolarized, and starlight is unpolarized. Visible/near-IR extinction and sub-mm emission polarization observations can help us infer magnetic field orientation.

Extinction describes the wavelength dependence of how dust blocks light. Blocking has two components: absorption and scattering. We can also observe thermal emission (describing the temperature peak) and microwave emission (describing spinning grains) and depletion. We'll focus on extinction first. Let's imagine we have some region of interest, and we're observing starlight through this region. To create extinction maps, we first identify nearby stars of a certain spectral type with no extinction, and we compare this to the stars with extinction. The extinction in magnitudes for some wavelength is given by

$$\frac{A_\lambda}{\text{mag}} = 2.5 \log_{10}\left[\frac{F_\lambda^0}{F_\lambda}\right] \tag{11.1}$$

where F_λ^0 is the flux without dust and F_λ is the observed flux. If we look at the same region at much longer wavelengths, we see that the light penetrates through this dust cloud.

From the equation of radiative transfer, we know that

$$\frac{F_\lambda^0}{F_\lambda} = e^{\tau_\lambda} \tag{11.2}$$

so we get

$$\frac{A_\lambda}{\text{mag}} = 2.5 \log_{10}[e^{\tau_\lambda}] = 1.086\tau_\lambda. \tag{11.3}$$

That is, optical depth and extinction in magnitudes are essentially the same number.

We can look at ratios of gas to dust: along most lines of sight in the galaxy, we have

$$\frac{N(H_{\text{tot}})}{A_v} = 1.9 \times 10^{21}\text{cm}^{-2}\text{mag}^{-1} \tag{11.4}$$

or

$$\frac{A_v}{N(H_{\text{tot}})} = 5.3 \times 10^{-22}\text{cm}^2\text{mag}. \tag{11.5}$$

Here, A_v denotes visual/visible extinction.

Even if we can't measure the flux directly, we can estimate the extinction by looking at the reddening/color excess. The "color" refers to the difference in magnitude at two different wavelengths. For example, we can compare the B band (4405 Å) and the V band (5470 Å). We have the *intrinsic color*,

$$(B - V)_0 = 2.5 \log_{10} \left(\frac{F_B^0}{F_V^0} \right) \tag{11.6}$$

and the *observed color*:

$$(B - V) = 2.5 \log_{10} \left(\frac{F_B}{F_V} \right). \tag{11.7}$$

The color excess is the intrinsic color minus the observed color:

$$E(B - V) = (B - V)_0 - (B - V) = 2.5 log_{10} \left(\frac{F_B^0/F_V^0}{F_B/F_V} \right). \tag{11.8}$$

So we have

$$\boxed{E(B - V) = A_B - A_V}. \tag{11.9}$$

We also look at the ratio $R_V = \frac{A_V}{A_B - A_V}$. R_V correlates positively with grain size.

We usually look at dust extinction curves, in which we plot A_λ normalized to a long wavelength over λ^{-1}. So we start at long wavelengths at which there's very little extinction and move to shorter ones where we expect more. There's usually a peak at 217.5 nm in these plots. The origin of this isn't well understood, but it's thought it isn't due to any particular chemical species.

If we have a dust grain of size a, we have a geometric cross-section of πa^2, an absorption cross-section $C_{\text{abs}}(\lambda)$, a scattering cross-section $C_{\text{sca}}(\lambda)$, and an extinction cross-section that's the sum of the last two:

$$C_{\text{ext}}(\lambda) = C_{\text{abs}}(\lambda) + C_{\text{sca}}(\lambda). \tag{11.10}$$

We often look at the albedo $\omega = \frac{C_{\text{sca}}}{C_{\text{ext}}}$.

We have

$$\tau_\lambda = N_{\text{dust}} C_{\text{ext}}(\lambda). \tag{11.11}$$

We have efficiency factors

$$Q_{\text{sca (abs)}} = \frac{C_{\text{sca (abs)}}}{\pi a^2} \tag{11.12}$$

where $a = \left(\frac{3V}{4\pi}\right)^{1/3}$.

To understand what happens within scattering, we look at three separate conditions on a relative to λ:

- $a \gg \lambda$ is geometric scattering;

- $a \sim \lambda$ is Mie scattering;

- $a \ll \lambda$ is Rayleigh scattering.

In this class we'll work in the Rayleigh scattering regime. We're interested in finding the scattering and absorption efficiency factors. Consider a dust grain with an EM field moving as a plane wave incident on it. A wave can be described as

$$E = E_0 \exp(i(kx - \omega t)). \tag{11.13}$$

k is the wavenumber and ω is the angular frequency. We have a dielectric constant $\varepsilon(\omega) = \varepsilon_1 + i\varepsilon_2$, and a refractive index $m = \sqrt{\varepsilon}$. A complex refractive index comes from field oscillations that are faster than the grain can move/polarize. So the response of the material can be out of phase with the EM field, causing extinction (why?)

$$k^2 = \epsilon(\omega)\frac{\omega^2}{c^2} \tag{11.14}$$

where $k = \frac{2\pi}{\lambda}$.

The spatial part of the E field goes as $E \propto e^{ikx} \propto e^{-(\operatorname{Im} k)x}$, and the intensity goes as the absolute value squared of the electric field, so

$$I \propto |E|^2 \propto e^{-2(\operatorname{Im} k)x}. \tag{11.15}$$

Also recall that $I \propto e^{-\tau_\lambda}$. So for a path of length L, we have an optical depth of

$$\tau = 2(\operatorname{Im} k)L. \tag{11.16}$$

We're guaranteed that $\operatorname{Im} k$ is positive because $\varepsilon_1, \varepsilon_2 > 0$ so the square root of ε has to live in the first quadrant.

Finally, we can calculate cross-sections:

$$C_{\text{sca}} = \int \frac{\mathrm{d}C_{\text{sca}}}{\mathrm{d}\Omega} \mathrm{d}\Omega = 24\pi^3 \left[\frac{(\varepsilon_1 - 1)^2 + \varepsilon_2^2}{(\varepsilon_1 + 2)^2 + \varepsilon_2^2} \right] \frac{V^2}{\lambda^4} \tag{11.17}$$

$$C_{\text{abs}} = 18\pi \frac{\varepsilon_2}{(\varepsilon_1 + 2)^2 + \varepsilon_2^2} \frac{V}{\lambda}. \tag{11.18}$$

The λ^{-4} dependence is characteristic of Rayleigh scattering.

As an example, consider an amorphous silicate feature with $\lambda = 10\mu$m. We have $\varepsilon = 0.996 + 2.575i$. Consider a graint with radius $a = 0.1\mu$m. We can compute $Q_{\text{abs}} = 0.124$ and $Q_{\text{sca}} = 1.77 \times 10^{-5}$. So absorption is about 7000 times more efficient than scattering.

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Diffuse Matter in Space **Fall 2023**

Lecture 12: Thermodynamics and composition of dust

Lecturer: Nia Imara *9 November* *Aditya Sengupta*

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12.1 Thermodynamics

Solid dust grains can interact with radiation at a wide wavelength range. This influences and is influenced by the thermodynamics of how dust grains behave.

Last time, we found that the optical depth due to dust was given by $\tau = 2 \operatorname{Im} kL$. To get absorption and scattering cross-sections, we derived expressions dependent on wavelength and optical depth.

Consider a population of spherical grains with radius a and number density n_{gr}. The absorption cross-section per grain at frequency ν is

$$C_{\mathrm{abs}} = Q_{\mathrm{abs}} \pi a^2 \tag{12.1}$$

and the attenuation coefficient is therefore

$$\kappa_\nu = n_{\mathrm{gr}} Q_{\mathrm{abs}} \pi a^2. \tag{12.2}$$

Internally, grains are generally in LTE, so

$$j_\nu = B_\nu(T) \kappa_\nu = n_{\mathrm{gr}} Q_{\mathrm{abs}} \pi a^2 B_\nu(T). \tag{12.3}$$

To compute the emission rate per unit volume, we integrate j_ν over all ν and directions, then divide by the number of grains in that volume (n_{gr}).

$$\left(\frac{\mathrm{d}E}{\mathrm{d}t}\right)_{\mathrm{emiss}} = 4\pi \int Q_{\mathrm{abs}}(\nu) \pi a^2 B_\nu(T) \mathrm{d}\nu. \tag{12.4}$$

To obtain energy absorption rate per unit volume, we do the same thing for $\kappa_\nu I_\nu$, where I_ν is the intensity of radiation incident on the grains:

$$\left(\frac{\mathrm{d}E}{\mathrm{d}t}\right)_{\mathrm{abs}} = \frac{1}{n_{\mathrm{gr}}} \int \kappa_\nu I_\nu \mathrm{d}\nu \mathrm{d}\Omega = \int \underbrace{h\nu}_{\text{energy per absorbed photon}} \underbrace{\frac{u_\nu}{h\nu} c Q_{\mathrm{abs}}(\nu \pi a^2)}_{n_{\mathrm{ph}} v \sigma} \, dd\nu. \tag{12.5}$$

We've used the energy density u_ν here.

We've seen that $Q_{\text{abs}} \sim \frac{2\pi a}{\lambda}$. For absorption (heating) it's convenient to define a spectrum-averaged absorption cross-section, weighted by the spectrum of radiation being absorbed.

$$\langle Q_{\text{abs}}\rangle_{\text{spec}} \equiv \frac{\int J_\nu Q_{\text{abs}}(\nu) dd\nu}{\int J_\nu d\nu}. \tag{12.6}$$

The radiative heating rate is then

$$\left(\frac{dE}{dt}\right)_{\text{abs}} = \langle Q_{\text{abs}}\rangle_* pi a^2 u_* c. \tag{12.7}$$

Here, $u_* = \int u_{*\nu} d\nu$ is the total radiation energy density.

For emission (cooling), we weight by the Planck function:

$$\langle Q_{\text{abs}}\rangle_T = \frac{\int B_\nu(T) Q_{\text{abs}} d\nu}{\int B_\nu(T) d\nu} \tag{12.8}$$

and so the cooling rate is

$$\left(\frac{dE}{dt}\right)_{\text{emiss}} = \langle Q_{\text{abs}}\rangle_T 4\pi a^2 \sigma T^4 \tag{12.9}$$

where σ is the Stefan-Boltzmann constant. Note that although we weight by the blackbody curve, this doesn't necessarily mean that the grain itself is a blackbody.

Taking the ratio of these, we can compare collisional and radiative heating:

$$\frac{(dE/dt)_{\text{col}}}{(dE/dt)_{\text{abs}}} = \frac{3.8 \times 10^{-6}}{U} \frac{\alpha}{\langle Q_{\text{abs}}\rangle_*} \frac{n_H}{30\text{cm}^{-3}} \left(\frac{T}{100\text{K}}\right)^{3/2}. \tag{12.10}$$

U is the radiation field strength normalized to the Milky Way average.

Collisions are unimportant in CNM and low-density regions, but collisional heating is important in dense and/or hot gas.

In steady state, emission and absorption are equal. We assume the spectrum of the interstellar radiation field, $Q_{\text{abs}} = Q_0(\lambda/\lambda_0)^{-\beta}$, and absorption properties of graphite and silicate material.

$$T \approx 16.4\left(\frac{a}{0.1\mu\text{m}}\right)^{-1/15} U^{1/6}\text{K}, \text{carbon}, 0.01 < (a/\mu\text{m}) < 1 \tag{12.11}$$

$$T \approx 22.3\left(\frac{a}{0.1\mu\text{m}}\right)^{-1/40} U^{1/6}\text{K}, \text{silicate}, 0.005 < (a/\mu\text{m}) < 0.15 \tag{12.12}$$

$$\tag{12.13}$$

So the grain temperature is largely insensitive to the radiation field, it's hard to heat up small dust grains, and grains do not radiate as blackbodies.

12.2   Composition

The overall abundances in the ISM are close to values in the solar photosphere, and H doesn't contribute appreciably to dust mass. Grains must form out of carbon, silicates, sulphur, and so on: light condensible materials.

Diffuse interstellar bands are weak emission lines seen in the optical whose origin is unclear. They are too broad to be absorption lines from atoms, ions, or small molecules. They might be ultra-small dust grains!

We also see polycyclic aromatic hydrocarbons (PAHs). Evidence of these is found in IR emission spectra. They generate emission at $\lambda = 3 - 13\mu$m.

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Diffuse Matter in Space **Fall 2023**

Lecture 13: H II regions

Lecturer: Nia Imara *14 November* *Aditya Sengupta*

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There are a few auxiliary types of ionization: Auger ionization, secondary ionization, and collisional ionization. But the main type of ionization in the ISM is photoionization, represented by

$$X + h\nu \rightarrow X^+ + e^-. \tag{13.1}$$

The rate of photoionization depends on a cross-section, which is a function of the frequency of light. The rate derivation is complicated and out of scope, so we'll just take it as a given. For a single-electron atom, the ionization cross-section for frequencies $\nu > Z^2 \frac{I_H}{h}$ is

$$\sigma_{pi} = \sigma_0 \left(\frac{Z^2 I_H}{h\nu} \right)^4 \frac{e^{4-(4\tan^{-1}x)x}}{1 - e^{-2\pi/x}} \tag{13.2}$$

where $x = \sqrt{\frac{h\nu}{Z^2 I_H} - 1}$, and

$$\sigma_0 = \frac{2^9 \pi}{3e^4} Z^{-2} \alpha \pi a_0^2 = 6.304 \times 10^{-18} Z^{-2} \text{cm}^2. \tag{13.3}$$

If we plot σ_{pi} as a function of $h\nu$, we start off with a ν^{-3} dependence, and later we get $\nu^{-3.5}$.

This gives us the ionization rate per atom,

$$\zeta_{pi} = \int_{\nu_0}^{\infty} \sigma_{pi}(\nu) 4\pi \frac{J_\nu}{h\nu} \mathrm{d}\nu. \tag{13.4}$$

Recombinations undo photoionization:

$$X^+ + e^- \rightarrow X + h\nu. \tag{13.5}$$

The rate of recombinations per unit time per unit volume is given by $n_p n_e \alpha$, where α is a recombination coefficient that is *not* the same as the fine structure constant.

Putting these two processes in equilibrium, we get

$$X_l + h\nu \leftrightarrow X_u^+ + e^-. \tag{13.6}$$

By the principle of detailed balance, we know the rates of photoionization and recombination have to be equal. We use $J_\nu = B_\nu$ in the ionization rate. Setting these equal, we get the *Milne relation*:

$$\sigma_{rr}(E) = \frac{g_l}{g_u} \frac{(I_{X,ul} + E)^2}{E m_e c^2} \sigma_{pi}(h\nu = I_{X,ul} + E). \tag{13.7}$$

Here, $I_{X,ul}$ is the difference in energy between ionized and unionized states. By integrating over the velocity distribution, this gives us a recombination rate,

$$\alpha_{nl}(T) = \left(\frac{8kT}{\pi m_e}\right)^{1/2} \int_0^\infty \sigma_{rr,nl}(E) x e^{-x} \mathrm{d}x. \tag{13.8}$$

Here, $x = E/kT$. We usually get α around $10^{-14} - 10^{-13} \mathrm{cm}^3 \mathrm{s}^{-1}$.

We have two cases of recombination: case A, the opticallly thin case where $T > 10^6$ K, and case B, the optically thick case which we have for H II.

For case A, we have

$$\alpha_A(T) = \sum_{n=1}^\infty \sum_{l=0}^{n-1} \alpha_{nl}(T) \tag{13.9}$$

which for H at 10^4K gives us

$$\alpha_A \approx 4.1 \times 10^{-13} \mathrm{cm}^3 \mathrm{s}^{-1}. \tag{13.10}$$

For case B, we have

$$\alpha_B(T) = \sum_{n=2}^\infty \sum_{l=0}^{n-1} \alpha_{nl}(T) = \alpha_A(T) - \alpha_{1s}(T). \tag{13.11}$$

For H at 10^4K, we have $\alpha_B \approx 2.5 \times 10^{-13} \mathrm{cm}^3 \mathrm{s}^{-1}$.

An example of what we can do with this is to estimate the cooling rate for a gas of pure fully-ionized H, at density n and temperature T. The KE of an electron on average is kT, so we can get a rate

$$\Lambda_{\mathrm{rec}} \sim \alpha_B n^2 kT. \tag{13.12}$$

A Strömgren sphere is a sphere of neutral ionized hydrogen around an O or B star. We assume a uniform medium with density n_H that is fully ionized. Let Q_0 be the rate of emission of photons having $h\nu geq 13.6$ eV. We require that the rates of photoionization and recombination are equal and we get a radius for the sphere,

$$R_s = \left(\frac{3Q_0}{4\pi\alpha_B n_H^2}\right)^{1/3} = 9.8 \times 10^{18} Q_{0,49}^{1/3} \left(\frac{n_H}{100\text{cm}^{-3}}\right)^{-2/3} \text{cm}. \tag{13.13}$$

Here, $Q_{0,49} = \frac{Q_0}{10^{49}}\text{s}^{-1}$.

If we had a star that suddenly turned on, what would the timescale to ionize the sphere? We have a number of particles given by $\frac{4}{3}\pi R_s^3 n_H$, and a rate of photon emission Q_0. Dividing these two simplifies to

$$t_{ion} = \frac{1}{\alpha_B n_H} = \frac{1200 \text{ years}}{(n_H/100\text{cm}^{-3})}. \tag{13.14}$$

So ionization equilibrium is established much faster than the timescale for evolution of a star off the main sequence.

We're interested in the fraction of ionized gas as a function of radius, for which we look at the Saha equation:

$$\boxed{\frac{\chi^2}{1-\chi} \approx \frac{1-y^3}{3y^2}\tau_s} \tag{13.15}$$

where $\chi = n_e/n_H$ is the fraction of ionized gas and $y = r/R_s$. We expect $\chi(y \to 0) = 1$ and $\chi(y \to \infty) = 0$.

Let's see how good our assumption of a fully ionized sphere is. The radius that encloses half the mass of the volume corresponds to $y = 2^{-1/3}$. At this radius, we have

$$\frac{\chi^2}{1-\chi} = 0.26\tau_s. \tag{13.16}$$

We can solve this as a quadratic equation, but in this case a linear expansion is okay:

$$1 - \chi \approx \frac{1}{0.26\tau_s} = 1.1 \times 10^{-3} Q_{0,49}^{-1/3} n_2^{-1/3}. \tag{13.17}$$

So the neutral fraction at half the mass is about one in a thousand, so being fully ionized is a good approximation.