Microphysical processes

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Collisional excitation and de-excitation

- In the previous lecture, we examined how atoms and molecules interact with the radiation field
- In this lecture, we will examine how they interact with each other (and with charged particles such as electrons) via collisions
- Collisions between particles can change the quantum state of one or both colliders (or leave them unchanged)
- Collisions can be treated fully quantum-mechanically using scattering theory. However, in this lecture we take a simpler approach

- We start by defining the collisional rate C_{ij}c
- This is the rate (per atom/molecule in state i) that collisions with some collider c cause a transition to state j
- Transition rate per unit volume = $C_{ij}^{c} n_{i}$
- To get the total collision rate C_{ij}, we simply sum over the rates for all possible collision partners:

$$C_{ij} = \sum_{c} C_{ij}^c.$$

- C_{ij}^c depends on n_c, the number density of collider c
- Useful to define a collisional rate coefficient q_{ij}^c that doesn't have this dependence:

$$q_{ij}^c \equiv \frac{C_{ij}^c}{n_c}.$$

 This in turn can be written as an integral of a velocitydependent collision cross-section over a velocity distribution:

$$q_{ij}^c = \int_0^\infty \sigma_{ij}^c(v) v f(v) \, \mathrm{d}v.$$

- The velocity distribution here is the distribution of relative velocities (at large distance) between the particle of interest and the collider c
- In the ISM, this is usually simply a Maxwell-Boltzmann distribution characterised by kinetic temperature T
- We will discuss approximate models for collisional crosssections this afternoon. For now, we assume that this is known (either from experiment or theory)

Given collisional coefficient for transition from i → j, the corresponding coefficient for the inverse reaction is:

$$q_{ji}^c = \frac{g_i}{g_j} q_{ij}^c e^{+E_{ij}/kT}$$

- This result follows from the principle of detailed balance
- In thermal equilibrium, transitions from i → j occur at same rate as transitions from j → i
- Therefore, in thermal equilibrium:

$$q_{ij}^c n_i n_c = q_{ji}^c n_j n_c.$$

• Rearranging this yields:

$$q_{ij}^c = q_{ji}^c \frac{n_j}{n_i}$$

 In thermal equilibrium, the ratio of n_j and n_i is given by a Boltzmann distribution:

$$\frac{n_j}{n_i} = \frac{g_j}{g_i} e^{-E_{ij}/kT},$$

 Substituting this into our expression for q_{ij} yields the desired relationship between q_{ij} and q_{ji}:

$$q_{ji}^c = \frac{g_i}{g_j} q_{ij}^c e^{+E_{ij}/kT}.$$

- Our derivation assumed thermal equilibrium
- However, we know that q_{ij}, q_{ji} just depend on the appropriate collision cross-section plus the velocity distribution
- Provided we have a Maxwell-Boltzmann velocity distribution, values of q_{ij}, q_{ji} don't depend on assumption of equilibrium
- Therefore, this relationship between collisional excitation, de-excitation holds in general, not only in equilibrium

The two-level atom

- We will explore interaction between collisional excitation, de-excitation and radiative effects using the simplest possible toy model: the two-level atom
- Lower level I, upper level u, energy separation Eul
- Start by assuming that any radiation field is negligible, so that we can ignore effects of absorption, stimulated emission
- NB. Necessary (but not sufficient) condition: gas must be optically thin otherwise $I_v \sim S_v$ locally

- Three effects that can change level populations: collisional excitation (C_{Iu}), collisional de-excitation (C_{ul}), radiative de-excitation (A_{ul})
- Level populations then evolve as:

$$\frac{\mathrm{d}n_u}{\mathrm{d}t} = C_{lu}n_l - C_{ul}n_u - A_{ul}n_u$$
$$\frac{\mathrm{d}n_l}{\mathrm{d}t} = -C_{lu}n_l + C_{ul}n_u + A_{ul}n_u$$

 In astrophysical context, characteristic timescale of these equations generally very short compared to other timescales of interest

- Therefore, usually OK to assume statistical equilibrium: individual atoms change level, but level populations remains constant
- In this case

$$C_{lu}n_l - C_{ul}n_u - A_{ul}n_u = 0$$
$$-C_{lu}n_l + C_{ul}n_u + A_{ul}n_u = 0$$

from which it follows that:

$$C_{lu}n_l = \left(C_{ul} + A_{ul}\right)n_u.$$

or alternatively:

$$\frac{n_u}{n_l} = \frac{C_{lu}}{C_{ul} + A_{ul}}.$$

• From detailed balance, we know that:

$$\frac{C_{lu}}{C_{ul}} = \frac{g_u}{g_l} e^{-E_{ul}/kT},$$

and so therefore:

$$\frac{n_u}{n_l} = \frac{(g_u/g_l)e^{-E_{ul}/kT}}{1 + A_{ul}/C_{ul}}.$$

- Key number here is the ratio of radiative de-excitation, collisional de-excitation rates, A_{ul} / C_{ul}
- If collisions dominate, A_{ul} / C_{ul} << 1 and we simply recover a Boltzmann distribution
- Conclusion: <u>when collisions dominate, the level</u> <u>populations are in LTE</u>
- If radiative de-excitations dominate, A_{ul} / C_{ul} >> 1 and hence n_u/n_l is much smaller than its LTE value

• In this regime — the low density regime — we have:

$$\frac{n_u}{n_l} \simeq \frac{C_{ul}}{A_{ul}} \frac{g_u}{g_l} e^{-E_{ul}/kT},$$

which we can also write as

$$\frac{n_u}{n_l} \simeq \frac{C_{lu}}{A_{ul}}.$$

(i.e. every collisional excitation is followed by a radiative de-excitation)

- Transition between two regimes occurs when $A_{ul} / C_{ul} = 1$
- Suppose C_{ul} dominated by collisions with one particular type of particle (e.g. electrons, H atoms, etc.)
- Then, at fixed temperature, C_{ul} varies linearly with density
- Can therefore identify one particular density for which we have $A_{ul} / C_{ul} = 1$ the **critical density** for the transition
- In terms of the collisional rate coefficient, this is:

$$n_{\rm cr}^c \equiv \frac{A_{ul}}{q_{ul}^c}.$$

- If q_{ul} varies with temperature, then so will critical density.
 However, this dependence is often fairly weak
- Different colliders have different q_{ul} and hence different critical densities. If more than one collision partner is important, overall critical density for transition will be:

$$n_{\rm cr} = \left[\sum_{c} \frac{x^c}{n_{\rm cr}^c}\right]^{-1},$$

 x_c is the fractional abundance of collider c

 Example: the [CII] 158 micron fine structure transition. This has a radiative transition rate:

$$A_{ul} = 2.4 \times 10^{-6} \,\mathrm{s}^{-1}$$

 In an ionized gas cloud (e.g. in the WIM), electron collisions dominate. For T > 2000 K, we have:

$$q_{ul} = 1.7 \times 10^{-6} T^{-0.345} \,\mathrm{cm}^3 \,\mathrm{s}^{-1}$$

• We therefore have a critical density:

$$n_{\rm cr} \simeq 30 \left(\frac{T}{10000 \,\mathrm{K}} \right)^{0.345} \,\mathrm{cm}^{-3}$$

In a neutral atomic gas cloud with x_e ~ 10⁻⁴ (e.g. a CNM cloud), collisions with H atoms dominate:

$$q_{ul} = 3.5 \times 10^{-11} T^{0.385} \text{ cm}^3 \text{ s}^{-1}$$

• In this case, the critical density is:

$$n_{\rm cr} \simeq 2000 \left(\frac{T}{10000 \,\mathrm{K}}\right)^{-0.385} \,\mathrm{cm}^{-3}$$

- Conclusions:
 - [CII] in low density limit in DIG ($n_e < 1 \text{ cm}^{-3}$)
 - [CII] in low n limit in CNM ($n_H < 100 \text{ cm}^{-3}$) and WNM
 - [CII] in LTE in some HII regions but not all typical HII region densities span wide range of values

- Variations in critical density primarily driven by differences in the value of A_{ul}
- This can vary by many orders of magnitude depending on transition energy, size of dipole moment, whether transition is permitted or forbidden, etc.
- Collisional de-excitation rates rarely vary by more than order of magnitude for given class of collisions (e.g. electrons with positive ions)
- For permitted optical/UV lines, critical densities are very large compared to ISM densities — low n limit applies
- For forbidden IR lines, critical densities much smaller, can find both low n, LTE behaviour

- Suppose now that the total number density of the atoms described by our two-level model is n_X
- From n_l + n_u = n_X plus our expression for n_u/n_l, we can derive the following relation:

$$\frac{n_u}{n_{\rm X}} = \frac{(g_u/g_l)e^{-E_{ul}/kT}}{1 + n_{\rm cr}/n + (g_u/g_l)e^{-E_{ul}/kT}}.$$

• When $n >> n_{cr}$, this reduces to:

$$\frac{n_u}{n_{\rm X}} = \frac{(g_u/g_l)e^{-E_{ul}/kT}}{Z(T)}$$

• Here, Z(T) is the **partition function** of the atom:

$$Z(T) = \sum_{i} \frac{g_i}{g_0} e^{-E_{i0}/kT}$$

- In high density limit, n_u depends purely on temperature and total number density of atoms
- Recall that we can write the emissivity as:

$$j_{\nu} = n_u A_{ul} \frac{h\nu}{4\pi} \phi_{\nu}.$$

- In LTE limit, emissivity is a linear function of density
- For an optically thin cloud in this limit:

$$I_{\nu} = \int j_{\nu} \, \mathrm{d}s.$$

• If cloud is also isothermal, then this simplifies to:

$$I_{\nu} = A_{ul} \frac{h\nu}{4\pi} \phi_{\nu} f_u N_{\rm X},$$

• Therefore, in the optically thin, LTE limit:

$$I_{\nu} \propto N_{\rm X}$$

- We can use <u>measured intensity</u> of line from some tracer to determine <u>column density</u> of that tracer provided:
 - Gas is optically thin
 - Tracer is in LTE
 - Gas is isothermal, with known temperature
- Last condition due to fact that we need to know fu
- Even if system not perfectly isothermal, not a large error if f_u does not vary strongly (e.g. HI 21 cm line: f_u ~ 3/4 with little dependence on T)

- Note that result holds regardless of density distribution within cloud, provided that tracer is in LTE
- This is hugely important often straightforward to determine gas temperature, difficult to determine density
- Optically thin condition can usually be ensured by choosing a tracer with a low chemical abundance (e.g. HCNO) or an isotopic variant of an abundant species (e.g. C¹⁸O)

 Given emissivity, we can also calculate <u>radiative cooling</u> <u>rate</u> per unit volume:

$$\Lambda_{ul} = \int \int n_u A_{ul} \frac{h\nu}{4\pi} \phi_{\nu} \, \mathrm{d}\nu \, \mathrm{d}\Omega,$$

= $n_u A_{ul} E_{ul},$

- In LTE limit, cooling rate depends on density of coolant, independent of density of collider
- Corollary: cooling time due to an LTE coolant is independent of density:

$$t_{\rm cool} = \frac{1}{\gamma - 1} \frac{nkT}{\Lambda_{ul}}$$

• In low density limit ($n \ll n_{cr}$), we have:

$$\frac{n_u}{n_{\rm X}} \simeq \frac{g_u}{g_l} e^{-E_{ul}/kT} \frac{n}{n_{\rm cr}}$$

 This can be written in terms of the collisional excitation rate coefficients as:

$$\frac{n_u}{n_{\rm X}} \simeq \frac{\sum_c q_{lu}^c x^c}{A_{ul}} n.$$

- In this limit, emission coefficient scales as n²
- Emission coefficient independent of A_{ul}: every collision results in emission of a photon, collisions are the rate-limiting step

- Consequence #1: measured intensity depends on integral of square of density, NOT on column density
- To compute this integral, we need to know the density distribution of the gas along the line of sight, which is information we generally don't have
- Consequence #2: radiative cooling rate becomes:

$$\Lambda_{ul} = E_{ul} \left(\sum_{c} q_{lu}^{c} n^{c} \right) n_{\mathbf{X}}.$$

Cooling limited by rate at which collisions occur, cooling time scales as $t_{cool} \sim n^{-1}$

H₂ cooling rate per molecule (Assumes H₂-H collisions dominate, 3:1 ortho-para mix)



- Cooling rate per atom/molecule increases with density until n ~ n_{cr}, thereafter remains constant
- Since different atoms/molecules have different critical densities, <u>dominant coolants vary with density even in</u> <u>absence of chemical evolution</u>



Neufeld et al (1995)

The effects of opacity

- What happens when the gas becomes optically thick?
- Since photons emitted in gas can't immediately escape, we can no longer ignore effects of the radiation field
- Therefore, need to redo our analysis of the two-level atom, retaining the absorption, stimulated emission terms

• In statistical equilibrium:

$$(C_{lu} + B_{lu}J_{ul})n_l = (A_{ul} + B_{ul}J_{ul} + C_{ul})n_u,$$

where:

$$J_{ul} = \frac{1}{4\pi} \oint I_{ul}(\vec{n}) d\Omega,$$

- Problem:
 - Level populations depend on Jul
 - Jul depends on Iul, which depends on level populations
- In principle, need to solve simultaneously for level populations and radiation field at every point in the gas!

- In practice, not possible for all but the simplest systems
- Numerical solutions typically adopt iterative approach:
 - Start with some guess for radiation field (e.g. Planck function with $T = T_{gas}$)
 - Use this to compute level populations
 - Solve RT problem with these level populations to obtain updated guess for radiation field
 - Repeat with new radiation field etc...
 - Stop iterating once level populations and radiation field have both converged within some specified tolerance

- For now, consider only a simple limiting case
- Assume external radiation field negligible and that photons emitted within the gas have only two fates:
 - Local absorption
 - Escape to infinity
- By "local", we mean within a region small enough that physical conditions (density, temperature etc.) are same as at point where photons are emitted
For photons of frequency v propagating in a direction n, the monochromatic escape probability is simply:

$$\beta(\vec{x}) = e^{-\tau_{\nu}(\vec{x},\vec{n})}$$

• To get the full escape probability, weight by line profile function and integrate over frequency and solid angle:

$$\langle \beta(\vec{x}) \rangle_{\Omega,\nu} = \frac{1}{4\pi} \int \int e^{-\tau_{\nu}(\vec{x},\vec{n})} \phi(\nu) d\nu \, d\Omega.$$

• When we refer simply to the **escape probability** for a line, we usually mean this more general expression

 Net local absorptions (i.e. absorption - stimulated emission) must balance number of emitted photons that do not escape:

$$(n_l B_{lu} - n_u B_{ul}) J_{ul} = n_u (1 - \beta) A_{ul}.$$

 Can use this to eliminate B coefficients from statistical equilibrium equation, resulting in:

$$C_{lu}n_l = (C_{ul} + \beta A_{ul})n_u.$$

- Same expression as in optically thin case, provided we make the substitution $A_{ul} \rightarrow \beta A_{ul}$
- System behaves as if A_{ul} were smaller effect known as photon trapping or radiative trapping
- Important consequence: n_{cr} also reduced by factor of β

What density does a given molecule line trace?

- You'll often see in textbooks or the astrophysical literature the statement that <u>molecular line emission traces</u> <u>densities close to n_{cr} for that particular line</u>
- When is this actually true?
- Emission per molecule scales with n for n << n_{cr}, constant for n >> n_{cr}
- Total emission from range of densities [n, n + δ n] is product of this with number of molecules in gas with density in this range

- Distribution of emission as function of density therefore depends on molecular abundance-weighted density probability distribution function (PDF)
- This describes fraction of total number of molecules we find at each density in gas
- If molecular abundance is independent of density, it is identical to the mass-weighted density PDF (i.e. function describing fraction of mass at each density)





- For constant or slowly decreasing density PDFs, emission mostly comes from n > n_{cr}
- For steeply decreasing density PDFs (e.g. log-normal), little emission from $n > n_{cr}$ (if larger than peak density)
- Molecular emission can trace densities far below n_{cr}
- Note: this effect is independent from the reduction in n_{cr} caused by high optical depth



Barnes et al (2020)



- "High density" tracers do not necessarily trace high densities — depends on density structure of cloud
- One important exception: N₂H⁺
- N₂H⁺ forms efficiently only once CO freezes out onto dust grains, hence only abundant in dense gas
- N₂H⁺ emission therefore traces dense gas much better than other commonly used tracers (e.g. HCN, HCO⁺)

Computing the escape probability

- In order for escape probability formalism to be useful, we obviously need to be able to compute β
- In general, this is a hard problem:
 - At each point, need τ for large number of angles
 - Computing each τ involves line integral of α
 - Need to repeat this for many points in cloud
 - For N fluid elements, cost scales as N^{5/3}

- For highly symmetric density fields, cost of computing β greatly reduced
- E.g. for a static slab, the average escape probability as a function of the optical depth of the slab is:

$$\beta_{\rm slab} = \frac{1 - {\rm e}^{-3\tau}}{3\tau}$$

• Doesn't fall off exponentially because:

1) We're averaging over whole slab

2) Optical depth in line wings much smaller than at line centre

- Similar expressions exist for spheres and various other simple geometries
- But real molecular clouds are not particularly spherical...



- Molecular clouds do appear to be highly turbulent
- Can therefore apply another useful approximation, the Large Velocity Gradient approximation
- Also known as the **Sobolev approximation**
- Basic idea: if there are large velocity differences between adjacent fluid elements, photons can escape more easily

- Consider photon emitted at point X with velocity V
- Suppose that this photon propagates to point X + Δ X, where velocity is V + Δ V
- What is likelihood of photon being absorbed at this point?
- Likelihood depends on size of ΔV compared to width of line if $\Delta V >>$ linewidth, absorption probability is small

 Quantify this by defining a characteristic length scale, the Sobolev length:

$$L_{\rm s} \equiv \frac{v_{\rm th}}{|dv/dx|},$$

Here, v_{th} is the thermal velocity of the absorber

- Note: expression for L_s implicitly assumes that velocity gradient is approx. constant on scale ~ L_s
- Photons that are able to propagate a distance L_s are likely to successfully escape from the gas

- LVG approximation: we assume that gas density, temperature, chemical composition etc. remain constant on scales < L_s
- Obviously, more likely to be valid when L_s is small, i.e. when velocity gradient is large
- Allows us to convert non-local problem into a local one of computing escape of radiation from small fluid element with constant density etc.

• In LVG approximation, escape probability becomes:

$$\beta(\vec{r},\vec{n}) = \frac{1 - e^{-\tau_{\rm LVG}}}{\tau_{\rm LVG}},$$

where:

$$\tau_{\rm LVG} = \frac{\alpha_0 c}{\nu_0 a_s} = \frac{A_{ul} c^3}{8\pi\nu_{ul}^3} \frac{1}{\left|\vec{n}\cdot\vec{\nabla}v\right|} \left(\frac{g_l}{g_u}n_u - n_l\right)$$

- Validity of LVG approximation depends on velocity gradients actually being large
- Good approximation in supersonically turbulent systems, such as GMCs
- Poor approximation in subsonic structures (e.g. prestellar cores), but often used anyway!

In most cases, interaction length comparable to size of smallest resolved structures (in simulations!)



Ossenkopf (2002)

Temperatures

- We finish up this lecture with a discussion of the different definitions of temperature that we may encounter
- Relation of this to our previous discussion of level populations will soon become apparent!
- Simplest definition: kinetic temperature (often just plain temperature, without qualifier) — temperature characterising small-scale thermal motions of particles
- Kinetic temperature is the T occurring in the Maxwell-Boltzmann distribution

- NB: We usually assume all types of particles located at some point in space have the same T (i.e. no separate temperatures for charged particles, neutrals)
- Good approximation in ISM (except for cosmic rays)
- However, other important quantities exist that are also referred to as "temperatures"
 - Excitation temperature
 - Brightness temperature
 - Antenna temperature

• Excitation temperature:

$$T_{\rm ex} \equiv \frac{E_{ul}}{k} \left[\ln \left(\frac{n_l g_u}{n_u g_l} \right) \right]^{-1}$$

• Rearranging this yields:

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} e^{-E_{ul}/kT_{\rm ex}}$$

 Excitation temperature describes level populations: <u>temperature of a Boltzmann distribution that would yield</u> <u>same values</u>

- In LTE, $T_{ex} = T$
- More generally:

$$\frac{T}{T_{\rm ex}} - 1 = \frac{kT}{E_{ul}} \ln\left(1 + \frac{n_{\rm cr}}{n}\right)$$

 When n << n_{cr}, T_{ex} << T. In this case, we often refer to the level populations as "subthermal" • Recall that the source function is:

$$S_{\nu} = \frac{n_u A_{ul}}{n_l B_{lu} - n_u B_{ul}}.$$

• Using relations between A_{ul}, B_{ul}, B_{lu}, can rewrite this as:

$$S_{\nu} = \frac{2h\nu_{ul}^{3}}{c^{2}} \left[\frac{n_{l}g_{u}}{g_{l}n_{u}} - 1 \right]^{-1}$$

• Therefore:

$$S_{\nu} = \frac{2h\nu_{ul}^3}{c^2} \left[\exp\left(\frac{E_{ul}}{kT_{ex}}\right) - 1 \right]^{-1}.$$

- For a cloud with constant T_{ex} , the source function is simply the Planck function with $T = T_{ex}$
- If the cloud is also optically thick, so that $I_v = S_v$, measuring I_v allows us to infer T_{ex}

- Brightness temperature: measure of strength of radiation field
- Brightness temperature T_b at a given frequency is the temperature of a Planck function producing same I_v at that frequency:

$$I_{\nu} = \frac{2h\nu^3/c^2}{e^{h\nu/kT_{\rm b}} - 1},$$

$$T_{b}^{-1} = \frac{k}{h\nu} \ln \left[1 + \frac{2h\nu^{3}}{c^{2}I_{\nu}} \right]$$

• In the **Rayleigh-Jeans** limit (hv << kT), this simplifies to:

$$T_{\rm b} = \frac{c^2}{2k\nu^2} I_{\nu}.$$

- In this limit (most commonly encountered in radio), the brightness temp. is a linear measure of intensity
- For an optically thick cloud, T_{ex} ~ T_b
- If the cloud is also in LTE, T ~ T_{ex} ~ T_{b}

- Antenna temperature: a measure of the power actually received by the telescope (usually in context of radio observations)
- Measured power = $k T_A$
- Related to brightness temperature of source by:

$$T_{\rm A} = \frac{\epsilon_r}{\Omega_{\rm A}} \int \int T_{\rm b}(\theta, \phi) P_n(\theta, \phi) d\theta d\phi,$$

- ε_r = transmission efficiency of antenna; usually ~ 1
- P_n = antenna power pattern



• Beam solid angle Ω_A is the integral of the antenna power pattern over the sky:

$$\Omega_{\rm A} = \int \int P_n(\theta, \phi) d\theta d\phi.$$

• If the solid angle subtended by the source (Ω_S) is much larger than Ω_A then:

$$T_{\rm A} \simeq \epsilon_r T_{\rm b}.$$

(assuming constant source brightness temperature)

• In this limit, can easily infer T_b from T_A

If source is small compared to beam (Ω_S << Ω_A), then we find instead that:

$$T_{\rm A} \simeq \epsilon_r \frac{\Omega_{\rm S}}{\Omega_{\rm A}} T_{\rm b}.$$

- Antenna temperature much smaller than source brightness temperature because of beam dilution
- Impact of this can be substantial, particularly for extragalactic observations

Detections of CO(3-2) line in WLM dwarf galaxy using APEX



Why are the measured brightness temperatures so small?

Elmegreen et al (2013)

 ALMA follow-up shows that each detection is actually a collection of compact clouds with angular sizes ~ 1"



 APEX beam size at frequency of CO(3-2) is ~ 18" — hence substantial beam dilution (factor of 18² ~ 300)

Summary

- In optically thin gas, easy to solve for level populations if we know collisional excitation, de-excitation rates and Einstein coefficients
- Analogous problem in optically thick gas much harder, as problem becomes non-local — generally need approximations such as LVG to solve
- Balance between collisional, radiative de-excitation quantified by critical density n_{crit}
- At densities n >> n_{crit}, level populations have LTE values
- In this high density regime, observed intensity traces column density (if tracer is optically thin)
- At densities n << n_{crit}, most atoms/molecules in their ground state
- In low density regime, observed intensity not a good tracer of column density
- Cooling rate per molecule scales with n in low density limit, tends to constant value as we approach n_{crit}

- Often quoted statement that "molecule emission traces gas with density close to n_{crit}" not always true — also sensitive to density distribution of cloud
- High optical depth implies radiative trapping, has effect of reducing effective critical density by factor of 1/β, where β = escape probability
- Many different temperatures we might refer to when discussing the ISM (kinetic, excitation, brightness, antenna) — important to understand the differences