# 400A - EOS (QM effects)

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**Materials**: Chapter 3 of Onno Pols' lecture notes, Chapter 14, 15, and 16 of Kippenhahn's book.

## Equation of state 2/2: Quantum-mechanical effects

In the previous lecture on EOS, we have discussed polytropic EOS and classical, non-relativistic, ideal gas. The latter is an accurate description of the stellar gas in most, but importantly not *all* the astrophysical cases.

We will consider now cases that don't verify the hypothesis we took previously and discuss briefly some stars for which we need to go beyond those.

A star is "big", why do we need to care about quantum mechanics (QM)? Besides its central role in allowing for nuclear burning, which we will see later, QM effects can matter also at extremely low temperatures and/or high densities, which can be encountered in stellar physics.

From the wave-nature of the solutions of Schroedinger's equation, we know that there is a limit on the precision to which position and velocity of a particle can be known ("Heisenberg's uncertainty principle"): $\Delta x \Delta p \geq h$ with $h$ Planck's constant. This naturally translates in three spatial dimension to

$$\Delta x \Delta y \Delta z \Delta p_x \Delta p_y \Delta p_z \geq h^3 \tag{1}$$

where $h^3$ is the volume of a quantized cell in phase-space! Thus the available number of quantized states with momentum between $p + dp$ within a volume $dV = dxdydz \equiv d^3x$ is

$$g(p)dpdV = g_s \frac{4\pi p^2 dpdV}{h^3} \text{ with } p = \sqrt{p_x^2 + p_y^2 + p_z^2}. \tag{2}$$

In the equation above, the factor $g_s$ allows to account for "internal degrees of freedom" of particles, e.g., their spin, polarization, or isospin. The key point here is $f(p) \propto p^2$ to satisfy QM. **N.B.:** the $p^2$ factor in $g(p)$ comes from the Jacobian from going from Cartesian to spherical polar coordinates in momentum space and assuming an isotropic momentum distribution ($dp_x dp_y dp_z \equiv d^3p = 4\pi p^2 dp$).

Let's start by considering a non-extreme situation. Then the particles are distributed according to a Maxwell-Boltzmann distribution $n(p)$, but whenever $n(p) > g(p)$, we know this is going to violate QM!

From the previous lecture on EOS we have already seen the Maxwell-Boltzmann distribution

$$n(p) \propto \frac{n}{(mT)^{3/2}} \exp\left(\frac{-p^2}{2mk_BT}\right) p^2 \quad , \tag{3}$$

where $n$ is the number density, $T$ the temperature, and $m$ the mass of the particles. Therefore:

$$\frac{n(p)}{g(p)} \propto n(mT)^{-3/2} \exp(\frac{-p^2}{2mk_BT}) \quad . \tag{4}$$

We can see that:

- at fixed temperature $T$, for very high number densities $n$, this ratio is going to be larger than one in violation of QM
- at fixed number density $n$, for very low temperatures $T$, this ratio will be larger than 1 in violation of QM (because every term in the Taylor expansion of the exponential is proportional to a negative power of $T$).
- the smaller mass particle will violate QM earlier than the higher mass particles

Thus, we can expect that for very "cold" stars (we will define what is the relevant scale here) or very dense stars the ideal gas EOS will not be appropriate.

To account for QM effects, we need to consider the nature of the particles making up the star, which can be either

- **Fermions** with semi-integer spin, such as electrons, protons, neutrons (and protons and neutrons can be seen as two different isospin states of a generic nucleon, this is useful for example to discuss the interior composition of neutron stars). In this case, the distribution function that determines the occupation of quantum states of energy between $\varepsilon \equiv \varepsilon(p)$ and $\varepsilon + d\varepsilon$ is the Fermi-Dirac distribution:

$$f_{FD}(\varepsilon) = \frac{1}{e^{(\varepsilon/k_B T - \eta)} + 1} \leq 1 \tag{5}$$

where $\eta = \mu/k_b T$ is the "degeneracy parameter" dependent on the *chemical potential* $\mu$, that is how much energy you need to "spend" to create a new particle in an available energy level (**N.B.:** do not confuse this with the mean molecular weight which has the same symbol, the chemical potential has the dimension of an energy, while the mean molecular weight is a dimensionless number!) and the temperature. The fact that this is $\leq 1$ is an expression of Pauli's exclusion principle, each quantized energy state can be occupied by at most one fermion.

- **Bosons** with integer spin, such as photons, or $\alpha$ particles. In this case the relevant distribution is the Bose-Einstein's distribution:

$$f_{BE}(\varepsilon) = \frac{1}{e^{(\varepsilon/k_B T - \eta)} - 1} \tag{6}$$

which can be $\geq 1$, meaning more than one boson can occupy the same energy level (e.g., in the extreme case of a Bose-Einstein condensate all particles occupy the level with lowest $\varepsilon$ - this may be relevant in the interior structure of neutron stars for example).

The total number of particles with momentum between $p$ and $p + dp$ is thus given by $f(\varepsilon(p))g(p)dp$ for an appropriate choice of $f$ depending on the particle considered ($f = f_{\mathrm{FD}}$ or $f = f_{\mathrm{BE}}$). To determine the chemical potential $\mu$ one can impose the normalization following from the total number density of particles:

$$n = \int_0^{+\infty} f(\varepsilon(p))g(p)dp \quad . \tag{7}$$

Let's now consider a gas of electrons. These are the particles in the ionized gas of the star that will first start feeling QM effects, since $m_e \ll m_{ion}$ (in fact $m_e \simeq m_{\mathrm{proton}}/1836.15 \simeq m_{proton}/2000$), cf. Eq. 4.

In practice, the pressure provided by the *ions* never becomes affected by QM directly: because of the $m^{-3/2}$ term in the Maxwell-Boltzmann distribution, this would require densities so high that the ions would not exist as ions anymore. Instead the high density would allow for electron captures onto the protons of the ions turning them in neutrons ($e^- + p \rightarrow n + \nu_e$). As we will see this is what happens at the very end of the evolution of massive stars that end their life exploding and leaving a neutron-star: those electron capture reactions are where the neutrons come from! The pressure provided by the neutrons does depend on QM effects and it is what sustains the structure of the neutron stars!

Because the pressure term from electrons (which in the ideal gas EOS is accounted for thanks to our definition of the mean molecular weight) changes because of QM effects first, let's now consider a gas made of electrons only. These particles have spin 1/2, thus they are fermions, and obey Eq. 5 and $q_s = 2$ in it (each quantum cell of the phase space $4\pi\ \mathrm{p}^2\mathrm{dp\ dV}$ can be occupied by 2 electrons, one with spin up and one with spin down).

## Fully degenerate electron gas

By definition, a fully degenerate gas is one where all the particles are in the lowest possible energy state, corresponding to the limit $\mathrm{T}\rightarrow 0$. Of course, if $\mathrm{T}\equiv 0$ there would be no cooling through radiation, the object would not be a *star* anymore (it would be if one wants a "black dwarf", a theoretical idea the Universe is too young to have produced, e.g., Caplan 2020). What we really mean by taking the $\mathrm{T}\rightarrow 0$ limit is that the thermal energy of the particles is very small compared to the Fermi energy: $\mathrm{k_b T} \ll \varepsilon_\mathrm{F}$. In this limit *the thermal and mechanical properties of the gas decouple from each other*, and we can assume $\mathrm{T} \simeq 0$ to discuss the mechanical properties, and consider T only for the radiative properties.

For fermions (like the electrons we are focusing on), this means that the electrons occupy a sphere in momentum space with a radius $\mathrm{p_F}$ called the "Fermi" momentum:

$$g_e(p)dp = q_s \frac{4\pi p^2}{h^3}dp \equiv \frac{8\pi p^2}{h^3}dp \ \text{ for } \ p \leq p_F \ \text{ otherwise } \ 0 \ , \qquad (8)$$

and we used $\mathrm{q_s}=2$ for electrons. To find the value of $\mathrm{p_f}$ we can use the normalization coming from the total number density of electrons

$$n_e = \int_0^{+\infty} g_e(p)dp = \frac{8\pi}{3h^3}p_f^3 \Rightarrow p_F = h\left(\frac{3}{8\pi}n_e\right)^{1/3} \quad . \qquad (9)$$

Therefore, the *Fermi momentum depends only on the density of electrons for a fully degenerate electron gas.*

We can now calculate the pressure exactly like we did for the classical ideal gas (cf. Eq. 12 in the Ideal gas section), we just need the appropriate p$\equiv$ p($\varepsilon$) relaton

### Non-relativistic electron gas

In this case $\varepsilon$ = $p^2/2m$ is the energy of the electrons (still ideal gas) and v=p/m, thus from the previous lecture on EOS we have:

$$P_e = \frac{1}{3}\int_0^{p_F} \frac{8\pi}{h^3}p^2\frac{p}{m_e}pdp = \frac{8\pi}{15h^3m_e}p_f^5 \equiv \frac{h^2}{20m_e}\left(\frac{3}{\pi}\right)^{2/3} n_e^{5/3} \quad . \tag{10}$$

Note the functional form $P_e \equiv P_e(n_e)$! It's a powerlaw, like we arbitrarily assumed would be a decent guess when discussing polytropes. *A fully degenerate classical electron gas has a polytropic EOS with exponent* $\Gamma$*=5/3.*

(to see this more explicitly you can use the definition of the electron mean molecular weight $\mu_e$ $n_e$ = $\rho/m_u$ to substitute $n_e$ for the mass density $\rho$).

### Ultra-relativistic electron gas

As the number density of electrons increases, $p_F$ increases, and thus at some point the v=p/m we used above will not hold anymore, because the electrons become relativistic. In the extremely relativistic limit, we can assume v=c (i.e. neglect the rest energy of the electrons in the p($\varepsilon$) relation), and then we lose one power of p in the integral above. Thus, in the *fully degenerate ultrarelativistic gas, the EOS will again be a polytrope with exponent now* $\Gamma$*=4/3.*

Specifically the calculation yields:

$$P_e = \frac{1}{3}\int_0^{p_F} \frac{8\pi}{h^3}p^2 cpdp = \frac{hc}{8}\left(\frac{3}{\pi}\right)^{1/3} n_e^{4/3} \quad . \tag{11}$$

In general, we should expect a **smooth** transition between these two polytopes as $n_e$ increases. Since the density in a star increases towards the center, we can expect this transition to occur as we move inwards in a star where these effects matter. In this case, we need to use the relativistic formula $p^2$ = $\varepsilon^2$-$m_e c^2$ to solve the integral and obtain the pressure.

One can estimate the density at the transition with the condition $p_F \simeq$ $m_e$ c:

$$\rho_{NR\to UR} \simeq \mu_e m_u \frac{8\pi}{3}\left(\frac{m_e c}{h}\right)^3 \quad . \tag{12}$$

### Partial degeneracy

The equations derived above are valid in the strict limit of T=0, necessary for **full** degeneracy. In reality it is sufficient to have $\mathrm{k_b T} \ll \varepsilon_\mathrm{F} = \mathrm{p_f}^2/2\mathrm{m}$ (for non-relativistic electrons). This is equivalent to asking $\eta \gg 1$ with $\eta$ electron degeneracy parameter.

The transition between ideal gas and fully degenerate gas goes through partially degenerate gas, and in that case the degeneracy pressure is harder to calculate analytically, and one needs to calculate $\mathrm{P} = 1/3 \times \int \mathrm{n(p)pvdp}$ using $\mathrm{n(p)} = \mathrm{g(p)f(\varepsilon(p))dp}$ with the Fermi-Dirac distribution for f (in the case of electrons).

For $\eta \ll 1$ the Fermi-Dirac distribution can be Taylor expanded and one recovers the ideal gas equation of state.

So, in summary, because electrons are Fermions that need to obey Pauli's principle at very low T (comparing their kinetic energy to the Fermi energy) and/or very high $\rho$, they can exert a much larger pressure than predicted by the classical ideal gas. Moreover, in those situation, the pressure is a polytrope, independent of temperature T! The decoupling between mechanical (hydrostatic structure) and radiative (energy transport) properties of the star afforded by degeneracy of the gas greatly simplifies the problem. This also means the stars do not need to heat up anymore in order to sustain themselves against their own gravity (breaking the conclusion we obtained from the Virial theorem). This is the situation of a "white dwarf" (WD), which are the remnants for the vast majority of stars, including the Sun.

These compact objects contract and cool until they fully crystallize (releasing further latent heat), becoming "planet-sized diamond-like structures"! In the homework you will also see how there is a maximum mass for a WD - the so-called Chandrasekhar mass, after the Nobel-prize winning discovery by Subrahmanyan Chandrasekhar.

### Radiation pressure

In some stars, the radiation field is so strong that is has a non-negligible contribution to the pressure. The particles providing that pressure are photons, which are **bosons** with 2 possible polarization states, so $\mathrm{q_S} = 2$ (in a classical electromagnetic wave language, this is because for a fixed propagation direction of a wave the electric field can still be in two directions, the two defining the plane orthogonal to the propagation direction).

Moreover, the number of photons does not need to be conserved, radiative processes will destroy/create photons as needed to achieve equilibrium: there is no chemical potential to overcome, thus $\eta$=0.

Finally, noting that the photons are ultra-relativistic by definition, we have $\varepsilon$ = pc = h$\nu$, and the Bose-Einstein distribution in Eq. 6 becomes the Black body distribution! We can then calculate the internal energy density of the photon gas as $\mathrm{u_{int}} = \mathrm{a\ T^4}$ with a the radiation constant:

$$a = \frac{8\pi^5 k_B^4}{15 h^3 c^3} = 7.56 \times 10^{-15} \mathrm{erg\ cm^{-3}\ K^{-4}} \quad , \tag{13}$$

which is closely related to the Stefan-Boltzmann constant $\sigma$: a=4$\sigma$/c.

Relying again on the ultra-relativistic nature of photons, we know that $\mathrm{P=u_{int}/3}$ and therefore the radiation pressure is:

$$P_{\mathrm{rad}} = \frac{1}{3} a T^4 \quad . \tag{14}$$

## Partial ionization effects

- **Q**: So far we have assumed full ionization of the gas. What do you think may change if we account for partial ionization? And where may that be important?

*Ionization is the process of removal of an electron from an ion*, which can be **collisional** (e.g., molecules/atoms bumping into each other in the atmosphere charging a cloud and preparing it for lightning discharge) or **radiative** (e.g., photoionization in the photoelectric effect that won Einstein the Nobel prize).

For an element with Z electrons there are Z+1 possible ions, from the neutral atom to the fully stripped nucleus with no electrons attached to it. For historical reasons, these are often indicated with the element symbol followed by a roman number from I - for the neutral atom to Z+1 in roman numbers for the fully ionized ion, e.g., HII for fully ionized hydrogen (cf. digression on spectra in the CMD/HRD lecture).

So far in our discussion of the EOS, we have considered always this last case of full ionization. Since the atomic binding energies are of order of ~1-10 eV (think of the Rydberg, $\chi$=13.6eV to strip Hydrogen of its electron from the fundamental state), that is $1\mathrm{eV}/\mathrm{k_B} \sim 10^4$ K, and most of the stellar material is hotter than this, this was probably not a bad approximation: the (thermal) kinetic energy of the particles flying around in the stellar gas are much larger than what is needed to separate electrons and ions, so probably this will happen a lot.

However, in the layers where T decreases, we can have partial ionization, which *will change the number of particles per unit atomic mass*, so you can expect this to *impact the mean molecular weight* $\mu$, and thus the pressure from the EOS (and we will see later also the temperature gradient).

By definition the mean molecular weight $\mu$ is such that $\rho = \mathrm{m_u}\mu(\mathrm{n}+\mathrm{n_e})$. This is what we used in the ideal gas equation to get $\mathrm{P}=\rho\ \mathrm{k_b T}/(\mu\ \mathrm{m_u})$ combining the electrons and ions pressure. Similarly we can define $\mu_0$ as the mean molecular weight per nucleus, and $\mu_\mathrm{e}$ as the mean molecular weight per electron, and thus

$$\rho = (n + n_e)\mu m_u \equiv n\mu_o m_u \equiv n_e\mu_e m_u \quad . \tag{15}$$

We can also define the number of free electrons per ion/atom $\mathrm{E}=\mathrm{n_e}/\mathrm{n}$ (where $\mathrm{n_e}$ is the number density of electrons and n the number density of massive ions regarless of their ionization state), and thus rewrite the above as

$$\mu = \frac{\rho}{m_u n}\frac{1}{1+E} \equiv \frac{\mu_0}{1+E} \equiv \mu_e\frac{E}{1+E} \quad . \tag{16}$$

which gives the relation between the mean molecular weight(s) and the number of free electrons. We will see in a later lecture how to calculate E as a function of T, and $\rho$.

## Total pressure in a generic star

Putting all things together:

$$P_\mathrm{tot} = P_\mathrm{gas} + P_\mathrm{rad} = \frac{\rho}{\mu m_u}k_B T + P_{QM} + \frac{1}{3}aT^4 \quad , \tag{17}$$

where we have decomposed the gas pressure into a degeneracy term due to quantum effects and a classical term.

Note that in practice, stellar evolution code often rely on *tabulated* EOS, which account for many non-ideal effects that we have only briefly discussed here. EOS are ultimately one of the points of contact between stellar physics and atomic physics and statistical mechanics:

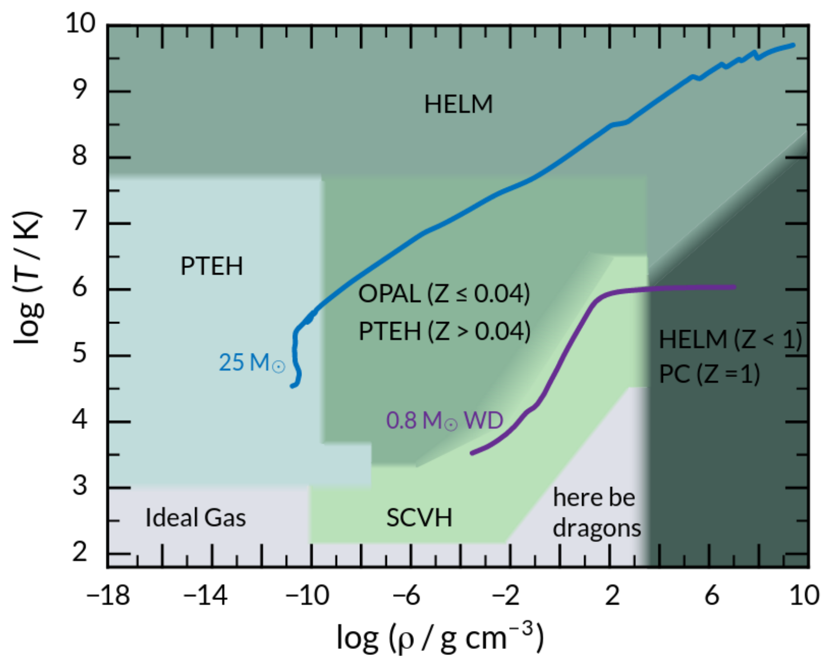


Figure 1: Blend of tabulated EOS on the T($\rho$) plane used in MESA (Fig. 50 in Paxton et al. 2018), see also Jermyn et al. 2021 for updates relevant to large portions of this plane. The blue and purple tracks correspond to evolved stellar models of the mass labeled.

A typical issue is how to obtain numerically good derivatives from tabulated EOS, especially at the boundaries between tables coming from different studies. These can often be a severe limiting factor in the numerical accuracy of stellar models, and this was one of the motivation for the development of a new EOS covering large portions of the T($\rho$) plane (Jermyn et al. 2021) now used by default in MESA.

## Homework

- Using the virial theorem, discuss which pressure term is more important in the total pressure as a function of the mass (and radius) of stars.

- Derive an upper limit for the temperature T as a function of the density $\rho$ for a star supported by fully degenerate (non-relativistic) electrons, and plot this relation on a $T(\rho)$ diagram. To explicit the relation between $n_e$ and $\rho$, assume a composition made of pure carbon ($X_i = 1$ if carbon, 0 otherwise, $Z_i = 6$, $A_i = 12$). Any T much lower than this limit can be considered $T \simeq 0$ for the purpose of the pressure calculation, but that still leaves a large range of non-zero T from the radiative point of view!

- Using the EOS for non-relativistic degenerate gas (and the other stellar equations you know), determine a mass-radius relation for stars entirely supported by (non-relativistic) electron degeneracy. This is a good approximation for a white dwarf, the end point of the vast majority (>98%) of stars!

- Clayton's problem 2-59: Let's now consider the case where electrons are are ultra-relativistic, show that the central pressure scales as $P_{center} \simeq 1.244 \times 10^{15}\ (\rho/\mu_e)^{4/3}$ dynes cm$^{-2}$. Consider the case where the electrons are ultra-relativistic *throughout* the star, then $P \simeq P_{center}$ *throughout* the star as well. Using the mass continuity equation and hydrostatic equilibrium, show that this implies that the only mass that the ultra-relativistic electron gas can sustain is $M_{Chandrasekhar} = 5.80\ M_\odot \times \mu_e^{-2} \simeq 1.44\ M_\odot$ for $\mu_e \simeq 2$ (note the $\mu_e^{-2}$ dependence!). What does this specific value of the mass (for a given composition, i.e., $\mu_e$) mean for stars supported by ultra-relativistic electron degeneracy pressure? What equation of stellar structure (of the ones we have seen so far) *cannot* be satisfied for larger values of the mass?