This week & next

Quantum degenerate gases – i.e., gases @ low temperature and/or high density,

where we can no longer ignore overlap of de Broglie waves.

Not to be confused w/ "degenerate energy levels"

① Before break we derived the Bose-Einstein & Fermi-Dirac distributions — today's focus

$$f_\pm(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} \pm 1}$$

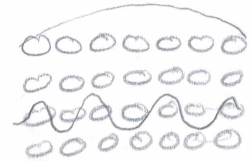
$+$ fermions

$-$ bosons

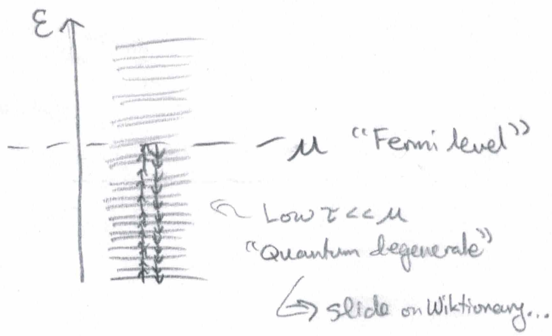
$f_\pm$ = occupation of a single eigenstate @ energy ε

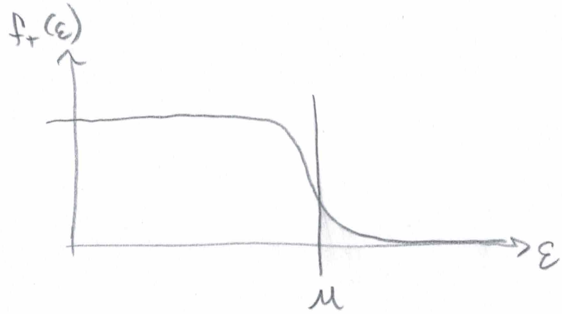
E.g. electrons in Cu: [Ar] 3d10 4s1

1 valence electron



Superpositions of s orbitals form energy bands:





⇒ Properties of metal (e.g. heat capacity, conductivity) are dictated by Fermi level μ

and density of states near Fermi level

Today: calculating $D(\varepsilon)$ for massive particles, relationship between Fermi level, total energy, # of particles

(e.g. conduction electrons, but also electrons in stars, etc...)

Quantum Degeneracy

degenerate

1. (*of qualities*) Having deteriorated, degraded or fallen from normal, coherent, balanced, and desirable to undesirable and typically abnormal.
2. (*of a human or system*) Having lost good or desirable qualities.

…

4. (*mathematics*) A degenerate case is a limiting case in which a class of object changes its nature so as to belong to another, usually simpler, class.
5. (*physics*) Having the same quantum energy level.

Wiktionary
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Derived terms

- (*physics*) degenerate matter

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EXERCISE 9A: FERMI DEGENERACY

define!

Objectives:

- Calculate the **density of states** of electrons in a metal
- Define and calculate the **Fermi energy**
- Examine the physical significance of the Fermi energy and **Fermi momentum**

References: Kittel & Kroemer, Ch. 7, pp. 181-199

Useful past results:

- Fermi-Dirac (+) and Bose-Einstein (−) distributions

$$f_{\pm}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} \pm 1}$$

describing the mean occupation of a single orbital of energy ε.

1. *Fermi Degeneracy.* Today, we will begin analyzing the implications of the Fermi-Dirac distribution for a realistic system with many orbitals characterized by a density of states $\mathcal{D}(\varepsilon)$, focusing on the regime of **quantum degeneracy**.

   a. List some physical systems can be modeled as gases of degenerate fermions.

Electrons in a metal

Electrons in a white dwarf star

Nuclear matter (protons & neutrons in nucleus)

Neutron stars

Liquid ^{3}He

Ultracold fermionic atoms (^{40}K, ^{6}Li, ..)

Differences

Non-relativistic or relativistic?

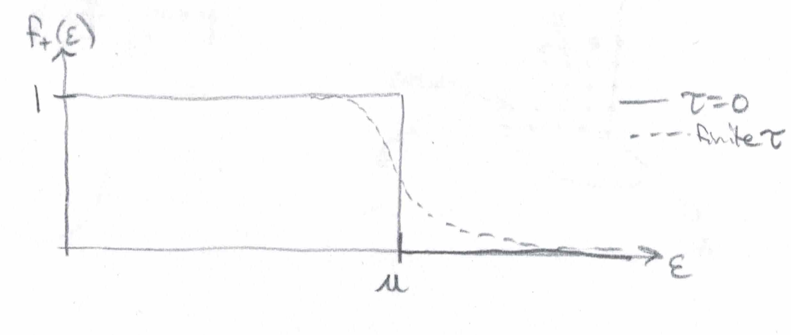
Interactions important or negligible?

Today: Focus on non-relativistic, non-interacting. Remarkably, this is a good approximation for conduction electrons in metals.

   b. For a gas of identical fermions, write down an integral expression for the particle number N in terms of the Fermi-Dirac distribution and the density of states.

$$N = \int_0^\infty d\varepsilon\, \mathcal{D}(\varepsilon)\, f_+(\varepsilon),$$

where



c. Simplify your expression in the zero-temperature limit $\tau \to 0$. The Fermi-Dirac distribution should drop out. What quantities determine N in this limit?

At $\tau = 0$, $f_+(\varepsilon) = \begin{cases} 1 & \text{for } \varepsilon < \mu \\ 0 & \text{for } \varepsilon > 0 \end{cases}$ (step function)

$$\Rightarrow N = \int_0^{\mu} d\varepsilon \, \mathcal{D}(\varepsilon)$$

$\Rightarrow$ N determined solely by Fermi level μ and density of states.

Even more simply, $N = \mathcal{N}(\mu)$
↑ total # of states up to Fermi level

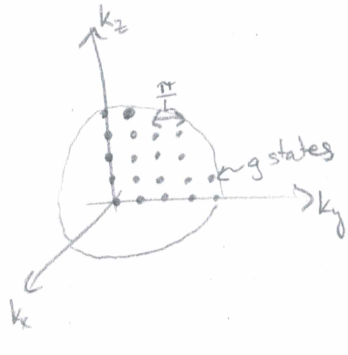
E.g., can treat e^-'s in metal (roughly) as particles in box b/c delocalized in superpositions of orbitals on different atoms

2. *Density of states for massive particles in a box.* Calculate the density of states $\mathcal{D}(\varepsilon)$ for a non-relativistic particle of mass m in a three-dimensional box of volume $V = L \times L \times L$. Allow for the possibility that the particle has g internal states that are independent of its spatial wave function (e.g., for a spin-1/2 particle, $g = 2$).

   a. We previously calculated the density of states $\mathcal{D}(\varepsilon)$ for photons and phonons. For purposes of such a calculation, what are the key similarities and differences between those systems and the gas of fermions?

   * Fermions are always massive vs. photons/phonons massless
     $\Rightarrow$ different dispersion relation $\varepsilon(k) = \frac{\hbar^2 k^2}{2m}$
   * Degeneracy g depends on spin; for spin-½, $g=2$ as for photons
   * Same form of wavefunction $\Psi \propto \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right)$, i.e., superpositions of plane waves w/ suitable boundary conditions

   b. The eigenstates can be visualized as a grid of points in **k**-space, where $\hbar\mathbf{k}$ is the momentum. Sketch this grid and indicate the spacing between the points in terms of L.



Spacing $\frac{\pi}{L}$

$\frac{n\lambda}{2} = L$

$k = \frac{2\pi}{\lambda} = \frac{2\pi n}{L \cdot 2} = \frac{\pi}{L}$

c. Calculate the following quantities in terms of the volume V:
   i. the number $\mathcal{N}(k)$ of quantum states of momentum $\leq \hbar k$
   ii. the number $\mathcal{N}(\varepsilon)$ of quantum states of energy $\leq \varepsilon$. — $\varepsilon = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \sqrt{2m\varepsilon}/\hbar$

i) $$\mathcal{N}(k) = \frac{g}{8} \cdot \frac{4}{3}\pi \left(\frac{k}{\pi/L}\right)^3 = \frac{gV}{6\pi^2} k^3$$

ii) $$\mathcal{N}(\varepsilon) = \frac{gV}{6\pi^2} \frac{(2m\varepsilon)^{3/2}}{\hbar^3} \equiv \alpha\, \varepsilon^{3/2}$$

d. Show that the density of states $\mathcal{D}(\varepsilon) = d\mathcal{N}/d\varepsilon$ is directly proportional to $\mathcal{N}/\varepsilon$, and find the constant of proportionality.
   i. Derive a relation between $d\mathcal{N}$ and $d\varepsilon$ by first relating $\ln \mathcal{N}$ to $\ln \varepsilon$.
   ii. Rearrange your expression from i. to obtain $\mathcal{D}(\varepsilon)$ in terms of $\mathcal{N}$ and ε.

i) $$\ln \mathcal{N} = \frac{3}{2}\ln \varepsilon + \underbrace{\ln\alpha}_{\text{const}}$$

$$\frac{1}{\mathcal{N}} d\mathcal{N} = \frac{3}{2\varepsilon} d\varepsilon \Rightarrow \boxed{\frac{d\mathcal{N}}{d\varepsilon} = \frac{3\mathcal{N}}{2\varepsilon} \equiv \mathcal{D}(\varepsilon)}$$

$$\Rightarrow \mathcal{D}(\varepsilon) = \frac{3}{2} \frac{gV}{6\pi^2} \frac{(2m)^{3/2}}{\hbar^3} \varepsilon^{1/2} \xrightarrow{g=2} \frac{V}{2\pi^2\hbar^3}(2m)^{3/2} \varepsilon^{1/2}$$ for spin-1/2

e. Evaluate $\mathcal{D}(\varepsilon)$ for a gas of spin-1/2 particles as a function of volume V, mass m, and energy ε.

See above: $\boxed{\mathcal{D}(\varepsilon) = \frac{V}{2\pi^2\hbar^3}(2m)^{3/2} \varepsilon^{1/2}}$

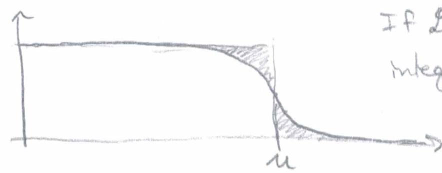
3. *Fermi energy and Fermi momentum.* The **Fermi energy** ε_F for a gas of N particles is defined by the relation

$$N = \int_0^{\varepsilon_F} \mathcal{D}(\varepsilon) d\varepsilon. \tag{1}$$

a. How is the **Fermi energy** related to the **Fermi level** (chemical potential) $\mu(n, \tau)$?

$\varepsilon_F = \mu(n, \tau = 0)$, i.e. the Fermi energy is the zero-temperature Fermi level. At finite temperature $\tau \ll \mu$, the Fermi energy and Fermi level (μ) are still the same to a good approximation;

$N = \int_0^\infty \mathcal{D}(\varepsilon) f_+(\varepsilon) d\varepsilon$



If $\mathcal{D}(\varepsilon)$ const. around μ, then integral is unchanged due to symmetry of Fermi-Dirac function about μ (HW problem).

b. Calculate the Fermi energy as a function of number density $n = N/V$ for a system of spin-1/2 fermions. Assume that ε_F is the same for both spin states.
Hint: use your calculation of $\mathcal{N}(\varepsilon)$ from part ~~iii~~ 2(c).

$$\mathcal{N}(\varepsilon_F) = N \Rightarrow \frac{V}{3\pi^2} \frac{(2m\varepsilon_F)^{3/2}}{\hbar^3} = N$$

$$(2m\varepsilon_F)^{3/2} = 3\pi^2\hbar^3 n \Rightarrow \varepsilon_F = (3\pi^2 n \hbar^3)^{2/3}/(2m)$$

$$\varepsilon_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

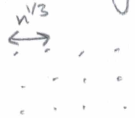
c. In terms of the Fermi energy ε_F, define the **Fermi momentum** $\hbar k_F = \sqrt{2m\varepsilon_F}$. Calculate $\hbar k_F$ in terms of the density n.

$$\hbar k_F = \sqrt{2m\varepsilon_F} = \hbar(3\pi^2 n)^{1/3}$$

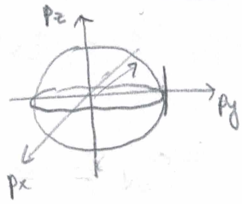
d. Explain the physical significance of the Fermi momentum in words and/or a sketch. (Real space? Momentum space?)

Real space

$n^{1/3}$ = interparticle spacing



Momentum space



occupied states fill a sphere of radius $\hbar k_F$

e. Calculate the de Broglie wavelength of particles at the Fermi level ε_F. Express it in terms of the interparticle spacing $n^{-1/3}$. How do you interpret your result?

$$\lambda_F = \frac{h}{p} = \frac{2\pi}{k_F} = \frac{2\pi}{(3\pi^2)^{1/3}} n^{-1/3} \propto \text{interparticle spacing}$$

* λ_F is the shortest wavelength of the occupied modes (@ low T) and thus dictates the smallest features in the density profile in real space, i.e. smallest possible period of modulations in e^- density.

* At low temperature, a single quantity ε_F describes characteristic energy and length scales.

We started part (f) and will discuss at start of next class.

f. Calculate the Fermi temperature $T_F = \varepsilon_F/k_B$ and the ratio T/T_F for the following systems:

i. A gas of electrons in copper at room temperature; the density of conduction electrons is $n = (0.23 \text{ nm})^{-3}$.

$$T_F = \frac{\hbar^2}{2mk_B}(3\pi^2 n)^{2/3} = 8\times 10^4 \text{ K}$$

$$T_{room} \approx 300 \text{ K} \Rightarrow \frac{T}{F_F} \approx 4\times 10^{-3}$$

ii. A white dwarf star composed of hydrogen atoms at a density $n = (1 \text{ pm})^{-3}$. At such a high density, the electrons are not bound to the protons; consider each in turn. The temperature of such a star is believed to be on the order of $T \sim 10^7$ K.

$$T_F^e = 4.2\times 10^9 \text{ K} \Rightarrow T/T_F^e \approx 0.2\times 10^{-2} = 2\times 10^{-3}$$

$$T_F^p = 2.3\times 10^6 \text{ K} \Rightarrow T/T_F^p \approx 4 \text{ — not degenerate}$$

* Electrons are degenerate but protons are not.
* Remarkably, electrons in copper are very similar to electrons in white dwarf star except for overall length scale (and, correspondingly, effects of gravity...)

iii. A spin-polarized gas of potassium-40 atoms at a density $n = (1\ \mu\text{m})^{-3}$ and a temperature of 10 nK.

First, why fermionic? ^{40}K has 19 protons, hence 19 e^-, 21 neutrons — all spin-1/2

Spin-polarized $\Rightarrow$ multiplicity $g=1$ (all same internal state).

$$\mathcal{N}_{g=1}(\varepsilon) = \tfrac{1}{2}\mathcal{N}_{g=2}(\varepsilon) \Rightarrow \varepsilon_F = \frac{\hbar^2}{2m}(6\pi^2 n)^{2/3} \Rightarrow \boxed{T_F = 91 \text{ nK}}$$

$\therefore T/T_F \approx 0.1 \Rightarrow$ degenerate

Not as deeply degenerate as electrons in a metal @ room temperature, despite being way colder!