

Problem Set 8

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1. Quantum densities for a non-relativistic ideal gas

The single-particle energies (in the non-relativistic limit) are quantized according to

$$E_{\underline{n}} = \frac{\hbar^2 \pi^2}{2mL^2} n^2 \quad (1)$$

where : in 1D : $\underline{n} \rightarrow n = 1, 2, 3, \dots$

in 2D : $\underline{n} \equiv (n_x, n_y)$, with $n = |\underline{n}| = \sqrt{n_x^2 + n_y^2}$
and $n_{x,y} = 1, 2, 3, \dots$

in 3D : $\underline{n} \equiv (n_x, n_y, n_z)$, with $n = |\underline{n}| = \sqrt{n_x^2 + n_y^2 + n_z^2}$
and $n_{x,y,z} = 1, 2, 3, \dots$

From Eq. (1), in the continuous limit,

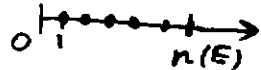
$$n(E) = \left(\frac{2m}{\hbar^2} \right) \frac{L}{\pi} \sqrt{E} \quad (\text{will use later}) \quad (2)$$

The density of single-particle orbitals is defined as

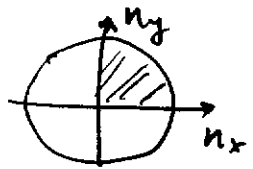
$$D(E) = \frac{\partial N(E)}{\partial E}$$

where $N(E)$ is the total number of states with energies less than E (including the spin states, i.e. $(2S+1)$ different values of the spin projection quantum number S_z for a given spin S)

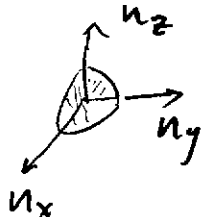
In 1D: $N(E) = (2S+1) \underbrace{n(E)}_{\text{from Eq. (2)}} = (2S+1) \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{L}{\pi} \sqrt{E}$



In 2D: $N(E) = (2S+1) \underbrace{\frac{1}{4} \pi n(E)^2}_{\substack{\text{area} \\ \text{in the} \\ \text{positive} \\ \text{quadrant}}} = (2S+1) \frac{1}{4} \pi \frac{2m}{\hbar^2} \left(\frac{L}{\pi} \right)^2 E$



In 3D: $N(E) = (2S+1) \underbrace{\frac{1}{8} \frac{4\pi}{3} n(E)^3}_{\substack{\text{volume} \\ \text{of the} \\ \text{positive} \\ \text{octant}}} = (2S+1) \frac{1}{8} \frac{4\pi}{3} \left(\frac{2m}{\hbar^2} \right)^{3/2} \left(\frac{L}{\pi} \right)^3 E^{3/2}$



Differentiating each of these $N(E)$ with respect to E , we obtain

$$D(E) = \frac{dN(E)}{dE} = \begin{cases} (2S+1) \frac{L}{2\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{1}{\sqrt{E}} & \text{— in 1D} \\ (2S+1) \frac{m A}{2\pi \hbar^2} & \text{— in 2D (where } A=L^2\text{)} \\ (2S+1) \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E} & \text{— in 3D (where } V=L^3\text{)} \end{cases}$$

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(a)

(i) in 1D : $N = (2S+1) n_F = 2 n_F$ → $S=1/2$ for electrons

$$\therefore n_F = \frac{N}{2}$$

$$E_F = \frac{\hbar^2}{2m} \left(\frac{\pi}{L} \right)^2 n_F^2 = \frac{\hbar^2}{2m} \left(\frac{\pi}{L} \right)^2 \left(\frac{N}{2} \right)^2 = \frac{\pi^2 \hbar^2 N^2}{8m L^2}$$

(ii) in 2D: $N = (2S+1) \cdot \frac{1}{4} \pi n_F^2 = \frac{1}{2} \pi n_F^2$ → $S=1/2$

$$\therefore n_F = \sqrt{2N/\pi}$$

$$E_F = \frac{\hbar^2}{2m} \left(\frac{\pi}{L} \right)^2 n_F^2 = \frac{\hbar^2}{2m} \frac{\pi^2}{A} \cdot \frac{2N}{\pi} = \frac{\pi \hbar^2 N}{m A}$$

→ $L^2 \equiv A$

(b) Total average energy of the gas, in general, is given by

$$U = \sum_{S_z} \sum_{\underline{n}} E_{\underline{n}} f_F(E_{\underline{n}}) = (2S+1) \sum_{\underline{n}} E_{\underline{n}} f(E_{\underline{n}})$$

→ Fermi-Dirac distr. fn.

$\underbrace{\sum_{S_z}}_{\text{spin projection (from } -S, -S+1, \dots, S-1, S)}$
 here $S=1/2$, so $S_z = \pm 1/2$

$$\rightarrow \begin{cases} (2S+1) \int_0^\infty dn E_n f_F(E_n), & \text{in 1D} \\ (2S+1) \frac{1}{4} 2\pi \int_0^\infty dn n E_n f_F(E_n), & \text{in 2D} \\ (2S+1) \frac{1}{8} 4\pi \int_0^\infty dn n^2 E_n f_F(E_n), & \text{in 3D} \end{cases}$$

or $\rightarrow \int_0^\infty dE D(E) E f_F(E)$
→ density of states in 1D, 2D or 3D

$$U = \int_0^{\infty} dE D(E) E f_F(E)$$

in 1D, 2D, or 3D

For a gas of electrons ($s=1/2$) in the ground state ($T=0$)

$$f_F(E) = \begin{cases} 1, & \text{if } E \leq E_F \\ 0, & \text{if } E > E_F \end{cases}$$

\therefore The ground state energy of the gas is:

$$U_0 = \int_0^{E_F} dE D(E) E \quad (\text{in 1D, 2D, or 3D})$$

(i) in 1D: $D(E) = \frac{L}{\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{1}{\sqrt{E}}$ \rightarrow from Problem 1, Problem Set 6 with $s=1/2$

$$\begin{aligned} \therefore U_0 &= \int_0^{E_F} dE \cdot E \cdot \frac{L}{\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{1}{\sqrt{E}} \\ &= \frac{L}{\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \int_0^{E_F} dE \sqrt{E} = \frac{L}{\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{2}{3} E_F^{3/2} \end{aligned}$$

Use the result of (a)-(i) that $E_F^{1/2} = \frac{\pi \hbar^2 N}{\sqrt{8m} L}$

$$\therefore U_0 = \frac{L}{\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{2}{3} \cdot E_F \cdot \underbrace{\frac{\pi \hbar^2 N}{\sqrt{8m} L}}_{E_F^{3/2}} = \frac{1}{3} N E_F$$

Thus
$$U_0 = \frac{1}{3} N E_F \quad \text{in 1D}$$

(ii) in 2D: $D(E) = (2s+1) \frac{mA}{2\pi\hbar^2} = \frac{mA}{\pi\hbar^2}$ (from problem 1, problem set 6)

$$\therefore U_0 = \int_0^{E_F} dE \cdot E \cdot D(E) = \frac{mA}{\pi\hbar^2} \int_0^{E_F} dE E = \frac{mA}{2\pi\hbar^2} E_F^2$$

Use the result of (a)-(ii) that $E_F = \frac{\pi\hbar^2}{mA} N$

$$\therefore U_0 = \frac{mA}{2\pi\hbar^2} E_F \cdot \frac{\pi\hbar^2}{mA} N = \frac{1}{2} N E_F$$

Thus $\boxed{U_0 = \frac{1}{2} N E_F}$ in 2D

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The density of copper (which I looked up in an introductory physics textbook) is 8.93 g/cm^3 , and the atomic mass (which I got off a periodic table) is 63.5 g/mol . Let's consider a chunk of copper containing one mole of atoms. Then the mass is 63.5 g , and the volume is

$$V = \frac{\text{mass}}{\text{density}} = \frac{63.5 \text{ g}}{8.93 \text{ g/cm}^3} = 7.11 \times 10^{-6} \text{ m}^3.$$

Assuming that each atom contributes one conduction electron, the number of conduction electrons per unit volume is

$$\frac{N}{V} = \frac{6.02 \times 10^{23}}{7.11 \times 10^{-6} \text{ m}^3} = 8.47 \times 10^{28} \text{ m}^{-3},$$

and therefore the Fermi energy is

$$\begin{aligned} \epsilon_F &= \frac{h^2}{8m} \left(\frac{3N}{\pi V} \right)^{2/3} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(9.11 \times 10^{-31} \text{ kg})} \left(\frac{3}{\pi} \cdot 8.47 \times 10^{28} \text{ m}^{-3} \right)^{2/3} \\ &= 1.13 \times 10^{-18} \text{ J} = 7.05 \text{ eV}. \end{aligned}$$

The Fermi temperature is just this divided by Boltzmann's constant,

$$T_F = \frac{\epsilon_F}{k} = \frac{7.05 \text{ eV}}{8.62 \times 10^{-5} \text{ eV/K}} = 82,000 \text{ K}.$$

This is 270 times greater than room temperature, so yes, room temperature is sufficiently low for this electron gas to be considered degenerate. The degeneracy pressure for this system is

$$P = \frac{2}{5} \frac{N}{V} \epsilon_F = (.4)(8.47 \times 10^{28} \text{ m}^{-3})(1.13 \times 10^{-18} \text{ J}) = 3.8 \times 10^{10} \text{ N/m}^2 = 3.8 \times 10^5 \text{ atm},$$

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To determine whether either approximation is valid, let's calculate the Fermi temperature for the electron gas at the center of the sun:

$$\begin{aligned} T_F &= \frac{\epsilon_F}{k} = \frac{h^2}{8mk} \left(\frac{3N}{\pi V} \right)^{2/3} = \frac{(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{8(9.1 \times 10^{-31} \text{ kg})(1.38 \times 10^{-23} \text{ J/K})} \left(\frac{3(10^{32} \text{ m}^{-3})}{\pi} \right)^{2/3} \\ &= 9.1 \times 10^6 \text{ K}. \end{aligned}$$

This is quite close to the actual temperature, of order 10^7 K . Since T is neither much greater than nor much less than T_F , neither approximation would be very accurate: We can't treat the gas as degenerate ($T \approx 0$), nor can we treat it as an ordinary "classical" ideal gas ($T \gg T_F$).