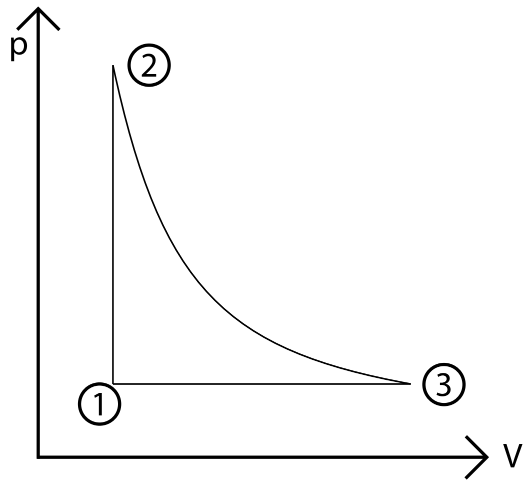
Prof. Dr. Roland Netz
Julius Schulz, Klaus Rinne

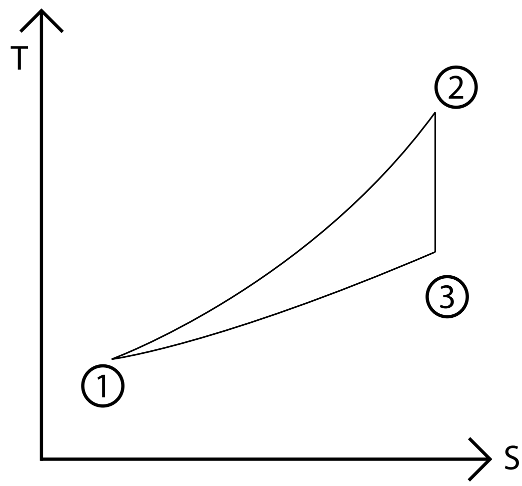
Exam Solutions: Advanced Statistical Physics
Part II: Problems (75P)

1 Lenoir Cycle (25P)

Consider 1 mol of an ideal gas, which initially has a volume V_1 and temperature T_1 at pressure p_1. The gas undergoes the following cyclic process:
$1 \to 2$: isochoric (constant V) heating to T_2
$2 \to 3$: isentropic expansion to V_3
$3 \to 1$: isobaric cooling

a) Sketch the P-V and the T-S diagram for this cyclic process. (6P)





$V_1 = V_2, p_1 = p_3$

b) For each step calculate the performed work W and the heat transfer Q in terms of p_1, V_1 and V_3. (15P)

$1 \to 2:$

$$W_{12} = \int_{V_1}^{V_2} p_1 \, \mathrm{d}V = 0, \quad \text{since } V_1 = V_2 \tag{1}$$

$$Q_{12} = c_V \, (T_2 - T_1) = c_V \, \frac{V_1}{R} \, (p_2 - p_1) = c_V \, \frac{V_1 \, p_1}{R} \left(\left(\frac{V_3}{V_1} \right)^{\gamma} - 1 \right) \tag{2}$$

using $p \, V = R \, T$ (ideal gas law) and $V_3^{\gamma} \, p_1 = V_2^{\gamma} \, p_2$ (adiabatic relation)

$$\tag{3}$$

$2 \to 3:$

$$Q_{23} = 0 \quad \text{(adiabatic process)} \tag{4}$$

$$W_{23} = c_V \, (T_2 - T_3) = U_2 - U_3 = \frac{c_V}{R} \, (p_1 \, V_3 - p_2 \, V_1) = \frac{c_V \, p_1}{R} \left(V_1 \left(\frac{V_3}{V_1} \right)^{\gamma} - V_3 \right) > 0 \tag{5}$$

$3 \to 1:$

$$W_{31} = \int_{V_3}^{V_1} p_1 \, \mathrm{d}V = p_1 \, (V_1 - V_3) \tag{6}$$

$$Q_{31} = W_{31} + U_1 - U_3 = (U_1 + p_1 V_1) - (U_3 + p_1 V_3) = H_1 - H_3 = c_P \, (T_1 - T_3) = -\frac{\gamma \, c_V \, p_1}{R} \, (V_3 - V_1) < 0 \tag{7}$$

c) Calculate the efficiency η in terms of $\alpha = V_3/V_1$. (4P)

$$\eta = \frac{W_{23} + W_{31}}{Q_{12}} = 1 + \frac{Q_{31}}{Q_{21}} = \frac{\alpha^\gamma - \alpha + \frac{R}{c_V}(1-\alpha)}{\alpha^\gamma - 1} = \frac{\alpha^\gamma - 1 + \gamma(1-\alpha)}{\alpha^\gamma - 1} = 1 - \gamma \frac{\alpha - 1}{\alpha^\gamma - 1} \tag{8}$$

2 Adsorption (25P)

Consider an ideal gas (temperature T, chemical potential μ) in contact with a surface with N adsorption sites. Each adsorption site may be occupied by 0, 1 or 2 gas molecules. The energy of a vacant site is zero, the energy with one adsorbed molecule is $-\epsilon$ and the energy with two adsorbed molecules is $-(3/2)\,\epsilon$. ϵ can be positive or negative. There is no interaction between molecules at different adsorption sites.

a) Calculate the grand canonical partition function for a fixed number N of adsorption sites. (10P)

$$\mathcal{Z}_1 = 1 + e^{\beta\,(\epsilon+\mu)} + e^{\beta\,(3\epsilon/2+2\mu)} \tag{9}$$

$$\mathcal{Z}_N = \mathcal{Z}_1^N \tag{10}$$

b) Use the grand canonical partition function to derive the mean number of adsorbed particles per site $\langle n \rangle$ and the mean internal energy per site $\langle u \rangle$ as a function of T, μ and ϵ. (8P)

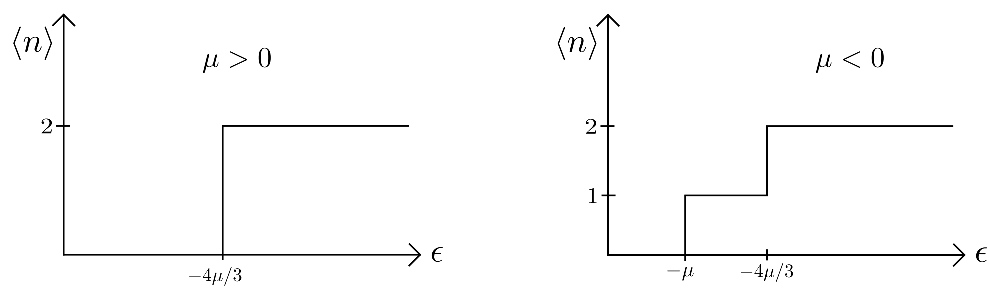
$$\langle n \rangle = \frac{1}{N} \frac{\partial(\ln \mathcal{Z}_N)}{\partial(\beta\,\mu)} \tag{11}$$

$$= \frac{e^{\beta(\epsilon+\mu)} + 2\,e^{\beta(3\epsilon/2+2\mu)}}{\mathcal{Z}_1} \tag{12}$$

$$\langle u \rangle = -\frac{1}{N}\left(\frac{\partial(\ln \mathcal{Z}_N)}{\partial \beta}\right)_{z,V} = -\frac{1}{N}\frac{\partial(\ln \mathcal{Z}_N)}{\partial\beta} + \mu\,\langle n \rangle \tag{13}$$

$$= -\frac{\epsilon\,e^{\beta(\epsilon+\mu)} + \epsilon\,\frac{3}{2}\,e^{\beta(3\epsilon/2+2\mu)}}{\mathcal{Z}_1} \tag{14}$$

c) For $T = 0$ sketch $\langle n \rangle$ for constant μ as a function of ϵ. (5P)



d) Calculate $\langle n \rangle$ for large temperatures. (No corrections in T are necessary.) (2P)

For large T and no corrections:

$$\beta \approx 0 \to \langle n \rangle = \frac{e^0 + 2\,e^0}{1 + e^0 + e^0} = \frac{1+2}{1+1+1} = 1 \tag{15}$$

3 Spin 1/2 Fermions in an External Magnetic Field in 2 Dimensions (25P)

Consider an ideal gas of N spin 1/2 Fermions at zero temperature confined to an area A in two dimensions. The Fermions are in an external magnetic field H. The energy of a particle is $\epsilon = \frac{p^2}{2m} \pm \mu_B H$, where μ_B is the Bohr magneton.

a) Give an expression for the chemical potential μ_0 for vanishing magnetic field as a function of the particle density N/A. (5P)

At $T = 0$ and for vanishing magentic field the chemical potential μ_0 equals the Fermi energy ϵ_F:

$$\mu_0 = \epsilon_F = \frac{p_F^2}{2m} \tag{16}$$

Since the Fermi-Dirac distribution is for $T = 0$ a step function we can integrate over a circle up to the Fermi momentum p_F:

$$\begin{aligned} N &= 2\frac{A}{h^2}\int_0^{p_F} \mathrm{d}^2p = 2\frac{A}{h^2}2\pi\int_0^{p_F} p\mathrm{d}p = 2\frac{A}{h^2}\pi p_F^2 \overset{(16)}{=} \frac{4\pi m A}{h^2}\mu_0 && (17)\\ \Leftrightarrow \mu_0 &= \frac{h^2 N}{4\pi m A} = \frac{1}{2m}\frac{h^2 N}{2\pi A} && (18) \end{aligned}$$

b) Calculate the average particle energy as a function of μ_0 for weak external magnetic fields. Calculate corrections in H up to second order. (14P)

For $H \neq 0$ the system has two Fermi momenta $p_\pm$:

$$\begin{aligned} \mu_0 &= \frac{p_\pm^2}{2m} \pm \mu_B H && (19)\\ \Leftrightarrow p_\pm &= \sqrt{2m\mu_0}\sqrt{1 \mp \mu_B H/\mu_0}, && (20) \end{aligned}$$

where p_- is the Fermi momenta of the spins oriented parallel to the external magnetic field H.

The total energy E_+ of the spins oriented anti-parallel to the external magnetic field is:

$$E_+ = \frac{A}{h^2}\int_0^{p_+} \epsilon_+ \mathrm{d}p^2 = \frac{2\pi A}{h^2}\int_0^{p_+}\left(\frac{p^2}{2m} + \mu_B H\right)p\mathrm{d}p = \frac{2\pi A}{h^2}\left(\frac{p_+^4}{8m} + \mu_B H\frac{p_+^2}{2}\right) \tag{21}$$

Analogously we find for the total energy E_- of the spins oriented parallel to the external magnetic field:

$$E_- = \frac{A}{h^2}\int_0^{p_-} \epsilon_- \mathrm{d}p^2 = \frac{2\pi A}{h^2}\int_0^{p_-}\left(\frac{p^2}{2m} - \mu_B H\right)p\mathrm{d}p = \frac{2\pi A}{h^2}\left(\frac{p_-^4}{8m} - \mu_B H\frac{p_-^2}{2}\right) \tag{22}$$

The average energy per particle E/N is:

$$\frac{E}{N} = \frac{E_+ + E_-}{N} = \frac{2\pi V}{h^2 N}\left(\frac{p_+^4 + p_-^4}{8m} + \mu_B H\frac{p_+^2 - p_-^2}{2}\right) \overset{(18)}{=} \frac{1}{2m\mu_0}\left(\frac{p_+^4 + p_-^4}{8m} + \mu_B H\frac{p_+^2 - p_-^2}{2}\right) \tag{23}$$

$$\frac{p_+^4 + p_-^4}{8m} = \frac{(2m\mu_0)^2}{8m}\left[(1 + \mu_B H/\mu_0)^2 + (1 - \mu_B H/\mu_0)^2\right] = 2m\mu_0\left[\mu_0/2 + (\mu_B H/\mu_0)^2\mu_0/2\right] \tag{24}$$

$$(p_+^2 - p_-^2)\mu_B H/2 \quad = \quad 2m\mu_0\mu_B H/2\,[1 - \mu_B H/\mu_0 - 1 - \mu_B H/\mu_0] = -2m\mu_0(\mu_B H/\mu_0)^2\mu_0 \tag{25}$$

By inserting equations (24) and (25) in equation (23) we determine the final result:

$$\frac{E}{N} \quad = \quad \mu_0/2 - (\mu_B H/\mu_0)^2\mu_0/2 \tag{26}$$

The first correction term reduces the average particle energy in second order of the strength of the applied magnetic field H.

c) Calculate the susceptibility $\chi = \partial m/\partial H$ for weak external magnetic fields. (6P)

The average number N_- of spins oriented parallel to the magnetic field is:

$$N_- \quad = \quad \frac{A}{h^2}\int\limits_0^{p_-} \mathrm{d}^2p = 2\pi\frac{A}{h^2}\int\limits_0^{p_-} p\mathrm{d}p = \frac{\pi A}{h^2}\pi p_-^2 = \frac{\pi A}{h^2}2m\mu_0(1 + \mu_B H/\mu_0) \overset{(18)}{=} \frac{N}{2}(1 + \mu_B H/\mu_0) \tag{27}$$

Analogously we find for the number N_+ of the spins oriented anti-parallel to the external magnetic field:

$$N_+ \quad = \quad \frac{N}{2}(1 - \mu_B H/\mu_0) \tag{28}$$

The average magnetisation m per area is:

$$m \quad = \quad \mu_B\frac{N_- - N_+}{V} = \frac{N\mu_B^2 H}{V\mu_0} \tag{29}$$

The susceptibility χ is:

$$\chi \quad = \quad \partial m/\partial H = \frac{N\mu_B^2}{V\mu_0} \tag{30}$$