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 → 2: isochoric (constant $V$) heating to $T_2$
2 → 3: isentropic expansion to $V_3$
3 → 1: isobaric cooling

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

\[ V_1 = V_2, \quad p_1 = p_3 \]

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 → 2:

\[ W_{12} = \int_{V_1}^{V_2} p_1 \, dV = 0, \quad \text{since } V_1 = V_2 \]  

(1)

\[ Q_{12} = c_v (T_2 - T_1) = c_v \frac{V_1}{R} (p_2 - p_1) = c_v \frac{V_1 p_1}{R} \left( \left( \frac{V_1}{V_2} \right)^\gamma - 1 \right) \]  

(2)

using $pV = RT$ (ideal gas law) and $V_3^\gamma p_1 = V_2^\gamma p_2$ (adiabatic relation)

(3)

2 → 3:

\[ Q_{23} = 0 \quad \text{(adiabatic process)} \]  

(4)

\[ W_{23} = c_v (T_2 - T_3) = U_2 - U_3 = c_v \frac{R}{p_1 V_1} (p_1 V_3 - p_2 V_1) = c_v \frac{p_1}{R} \left( V_1 \left( \frac{V_3}{V_1} \right)^\gamma - V_3 \right) > 0 \]  

(5)
3 \rightarrow 1:\n
\[ \begin{align*}
W_{31} &= \int_{V_3}^{V_1} p_1 \, dV = p_1 (V_1 - V_3) \\
Q_{31} &= W_{31} + U_1 - U_3 = (U_1 + p_1 V_1) - (U_3 + p_1 V_3) = H_1 - H_3 = c_p (T_1 - T_3) = -\frac{\gamma c_v p_1}{R} (V_3 - V_1) < 0
\end{align*} \] (6)

(7)

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

\[ \eta = \frac{W_{23} + W_{31}}{Q_{12}} = 1 + \frac{Q_{31}}{Q_{21}} = \frac{\alpha \gamma - \alpha + R}{\alpha \gamma - 1} = \frac{\alpha \gamma - 1 + \gamma (1 - \alpha)}{\alpha \gamma - 1} = 1 - \gamma \frac{\alpha - 1}{\alpha \gamma - 1} \] (8)

2 Adsorption (25P)

Consider an ideal gas (temperature \( T \), chemical potential \( \mu \)) 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 \( -(3/2) \epsilon \). \( \epsilon \) 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)

\[ Z_1 = 1 + e^{\beta(\epsilon + \mu)} + e^{\beta(3\epsilon/2 + 2\mu)} \] (9)

\[ Z_N = Z_1^N \] (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 \( T, \mu \) and \( \epsilon \). (8P)

\[ \langle n \rangle = \frac{1}{N} \frac{\partial \ln Z_N}{\partial(\beta \mu)} = \frac{e^{\beta(\epsilon + \mu)} + 2 e^{\beta(3\epsilon/2 + 2\mu)}}{Z_1} \] (11)

\[ \langle u \rangle = -\frac{1}{N} \left( \frac{\partial \ln Z_N}{\partial \beta} \right)_{T,V} = -\frac{1}{N} \frac{\partial \ln Z_N}{\partial \beta} + \mu \langle n \rangle = -\epsilon e^{\beta(\epsilon + \mu)} + \epsilon^2 e^{\beta(3\epsilon/2 + 2\mu)} \] (12)

\[ \langle u \rangle = -\epsilon e^{\beta(\epsilon + \mu)} + \epsilon^2 e^{\beta(3\epsilon/2 + 2\mu)} \] (13)

\[ \langle u \rangle = -\epsilon e^{\beta(\epsilon + \mu)} + \epsilon^2 e^{\beta(3\epsilon/2 + 2\mu)} \] (14)

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

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

For large \( T \) and no corrections:

\[ \beta \approx 0 \rightarrow \langle n \rangle = \frac{e^0 + 2 e^0}{1 + e^0 + e^0} = \frac{1 + 2}{1 + 1 + 1} = 1 \] (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 \( \mu_B \) is the Bohr magneton.

a) Give an expression for the chemical potential \( \mu_0 \) for vanishing magnetic field as a function of the particle density \( N/A \). (5P)

At \( T = 0 \) and for vanishing magnetic field the chemical potential \( \mu_0 \) equals the Fermi energy \( \epsilon_F \):

\[
\mu_0 = \epsilon_F = \frac{p_F^2}{2m}
\]  

(16)

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

\[
N = 2 \frac{A}{\hbar^2} \int_0^{p_F} \frac{d^2p}{2\pi} = \frac{2A}{\hbar^2} \pi p_F^2 = \frac{4\pi m A}{\hbar^2} \mu_0
\]  

(17)

\[
\Rightarrow \mu_0 = \frac{\hbar^2 N}{4\pi mA} = \frac{1}{2m} \frac{h^2 N}{2\pi A}
\]  

(18)

b) Calculate the average particle energy as a function of \( \mu_0 \) for weak external magnetic fields. Calculate corrections in \( H \) up to second order. (14P)

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

\[
\mu_0 = \frac{p_\pm^2}{2m} \pm \mu_B H
\]  

(19)

\[
\Rightarrow p_\pm = \sqrt{2m\mu_0} \sqrt{1 \pm \mu_B H/\mu_0},
\]  

(20)

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:

\[
E_+ = \frac{A}{\hbar^2} \int_0^{p_+} \epsilon_+ dp = \frac{2\pi A}{\hbar^2} \int_0^{p_+} \left( \frac{p^2}{2m} + \mu_B H \right) dp = \frac{2\pi A}{\hbar^2} \left( \frac{p_+^4}{8m} + \mu_B H \frac{p_+^2}{2} \right)
\]  

(21)

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

\[
E_- = \frac{A}{\hbar^2} \int_0^{p_-} \epsilon_- dp = \frac{2\pi A}{\hbar^2} \int_0^{p_-} \left( \frac{p^2}{2m} - \mu_B H \right) dp = \frac{2\pi A}{\hbar^2} \left( \frac{p_-^4}{8m} - \mu_B H \frac{p_-^2}{2} \right)
\]  

(22)

The average energy per particle \( E/N \) is:

\[
\frac{E}{N} = \frac{E_+ + E_-}{N} = \frac{2\pi V}{\hbar^2 N} \left( \frac{p_+^4}{8m} + \mu_B H \frac{p_+^2}{2} + \frac{p_-^4}{8m} - \mu_B H \frac{p_-^2}{2} \right) = \frac{1}{2m\mu_0} \left( \frac{p_+^4}{8m} + \frac{p_-^4}{8m} + \mu_B H \frac{p_+^2}{2} - \mu_B H \frac{p_-^2}{2} \right)
\]  

(23)

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

(24)
\[(p^2_+ - p^2_-)\mu_B H/2 = 2m\mu_0\mu_B H/2 [1 - \mu_B H/\mu_0 - 1 - \mu_B H/\mu_0] = -2m\mu_0(\mu_B H/\mu_0)^2\mu_0 \quad (25)\]

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

\[\frac{E}{N} = \mu_0/2 - (\mu_B H/\rho_0)^2\mu_0/2 \quad (26)\]

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:

\[N_- = \frac{A}{\hbar^2} \int_0^{p_-} d^2p = 2\pi \frac{A}{\hbar^2} \int_0^{p_-} pdp = \pi A \frac{\hbar^2}{\hbar^2} \pi p^- = \pi A \frac{\hbar^2}{\hbar^2} 2m\mu_0(1 + \mu_B H/\mu_0) = \frac{N}{2}(1 + \mu_B H/\mu_0) \quad (27)\]

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

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

The average magnetisation \(m\) per area is:

\[m = \mu_B \frac{N_- - N_+}{V} = \frac{N\mu_B^2 H}{V\mu_0} \quad (29)\]

The susceptibility \(\chi\) is:

\[\chi = \partial m/\partial H = \frac{N\mu_B^2}{V\mu_0} \quad (30)\]