SAMPLE SOLUTIONS EXERCISE 12

EXERCISE 12.1: COMBUSTION MOTOR (4P)

Estimate the thermodynamic cycle in a petrol engine assuming an ideal gas in a quasi-static approximation.

- $A \to B$: Adiabatic compression from volume V_A to volume V_B.
- $B \to C$: The explosion increases the pressure by Δp.
- $C \to D$: Adiabatic expansion from volume V_B to volume V_A.
- $D \to A$: Cooling of the gas at constant volume.

An ideal gas obeys the state equation $E = \frac{3}{2}pV = \frac{3}{2}Nk_BT$.
An ideal gas expands/compresses adiabatically along the adiabatic lines $pV^{5/3} = const.$

(a) Sketch the cyclic process in a (p, V) diagram as well as in a (H, V) diagram. (1P)

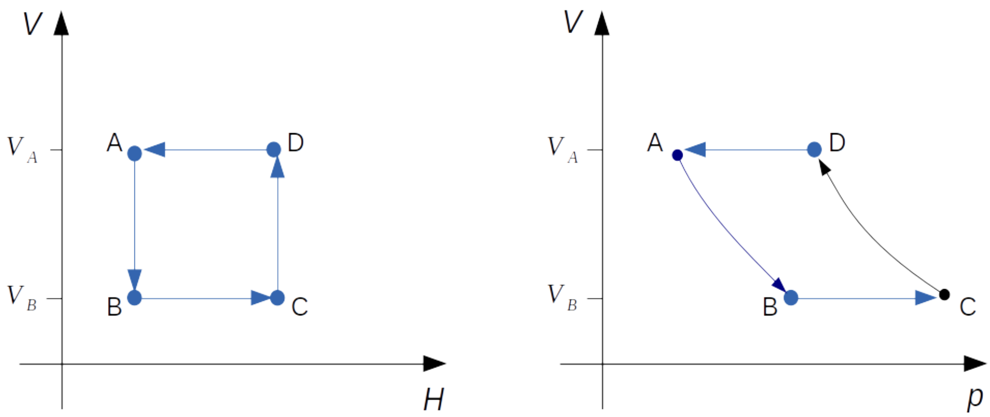
(b) Compute the work during adiabatic compression and expansion. (1P)

(c) Show that the efficiency of the machine in a whole cycle is given by (2P)

$$\eta = \frac{\Delta W}{\Delta Q} = 1 - \left(\frac{V_B}{V_A}\right)^{\frac{2}{3}}$$

SAMPLE SOLUTION

(a) The cycles are:



(b) **1. ADIABATIC COMPRESSION $A \to B$:**
During compression from A to B the volume change is negative ($\mathrm{d}V < 0$) and hence the work $\mathrm{d}W = p\,\mathrm{d}V$ is negative (meaning that we have to perform work to compress the gas):

$$\Delta W_{A\to B} = \int_{V_A}^{V_B} p(V)\,\mathrm{d}V = -\int_{V_B}^{V_A} p(V)\,\mathrm{d}V < 0$$

Along adiabatic lines we have $p(V)V^\kappa = const$, where $\kappa = 5/3$ for the ideal gas. This means that

$$p(V) = p_A \left(\frac{V_A}{V}\right)^\kappa$$

Inserting this into the above integral we get the work

$$\Delta W_{A\to B} = \frac{p_A V_A}{\kappa - 1}\left(1 - \left(\frac{V_A}{V_B}\right)^{\kappa-1}\right) < 0$$

(c) **2. EXPLOSION OF THE FUEL $B \to C$:**
The burning process increases the internal energy E of the gas by ΔQ (converting chemical into thermal energy). Since the volume V_B is constant, the caloric equation of state of the ideal gas $E = \frac{3}{2}pV$ tells us that there will be an increase of the pressure by

$$p_C = p_B + \Delta p\,, \qquad \Delta p = \frac{2\Delta Q}{3V_B}$$

3. ADIABATIC EXPANSION $C \to D$:
Analogous to compression, but now the work is positive:

$$\Delta W_{C\to D} = \frac{p_C V_B}{\kappa - 1}\left(1 - \left(\frac{V_B}{V_A}\right)^{\kappa-1}\right) > 0$$

4. COOLING $D \to A$:
Cooling at constant volume brings the pressure back to p_A. We do not need to calculate this explicitly.

PUTTING ALL THINGS TOGETHER:
The efficiency of the engine is defined as

$$\eta = \frac{\Delta W_{A\to B} + \Delta W_{C\to D}}{\Delta Q}$$

Inserting the formulas and using $p_A V_A^\kappa = p_B V_B^\kappa$ we arrive at

$$\eta = \frac{p_A V_A \left(1 - \left(\frac{V_A}{V_B}\right)^{\kappa-1}\right) + (p_B + \Delta p)V_B\left(1 - \left(\frac{V_B}{V_A}\right)^{\kappa-1}\right)}{(\kappa-1)\frac{3}{2}\Delta p V_B} = 1 - \left(\frac{V_B}{V_A}\right)^{\frac{2}{3}}\,.$$

EXERCISE 12.2: QUANTUM PARTICLE IN A 1D POTENTIAL WELL (8P)

Let us consider a single quantum-mechanical particle in a one-dimensional infinite potential well of length L in contact with a thermal reservoir at temperature T.

(a) Compute the energy eigenvalues and write down the partition sum. (1P)

(b) Show that in the low-temperature limit $T \to 0$ the logarithm of the partition sum is given by leading and next-to-leading order by (2P)

$$\ln Z(\beta, L) = -\frac{\beta\gamma}{L^2} + e^{-3\frac{\beta\gamma}{L^2}} + \mathcal{O}\big(e^{-8\frac{\beta\gamma}{L^2}}\big) \quad \text{where} \quad \gamma = \frac{\pi^2\hbar^2}{2m}.$$

(c) Compute the average energy E, the heat capacity C, and the pressure P in the limit of low temperatures by calculating the corresponding derivatives of $\ln Z$. (1P)

(d) Why is $P > 0$ in the limit $T \to 0$? (1P)

(e) Approximate the partition sum in the high-temperature limit $T \to \infty$. (2P)

(f) Compute E, C, and P in the limit of high temperatures. (1P)

Sample Solution

(a) We are looking for the solutions of the stationary Schrödinger equation $-\frac{\hbar^2}{2m}\Delta\psi(x) = E\psi(x)$ obeying the Dirichlet boundary conditions $\psi(0) = \psi(L) = 0$ at the infinite potential well. With the ansatz $\psi(x) \propto \sin(kx)$ we find that the wave numbers are quantized in steps of $k = n\pi/L$ where $n = 1, 2, \ldots$. Inserting this ansatz into the Schrödinger equation gives the energies

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}.$$

This allows us to formally write down the partition sum

$$Z(\beta, L) = \sum_{n=1}^{\infty} e^{-\frac{\beta\gamma n^2}{L^2}} \quad \text{where} \quad \gamma = \frac{\pi^2\hbar^2}{2m}, \quad \beta = \frac{1}{T}.$$

Unfortunately, this partition sum cannot be evaluated explicitly, and this is why we will study approximations below.

(b) In the limit $T \to 0$ we have $\beta \to \infty$, hence $e^{-\beta\gamma/L^2}$ is very small. Thus, the partition sum Z can be approximated to leading and next-to-leading order by

$$Z(\beta, L) = e^{-\frac{\beta\gamma}{L^2}} + e^{-\frac{4\beta\gamma}{L^2}} + \ldots = e^{-\frac{\beta\gamma}{L^2}}\left(1 + e^{-\frac{3\beta\gamma}{L^2}} + \ldots\right).$$

$$\Rightarrow \quad \ln Z(\beta, L) = -\frac{\beta\gamma}{L^2} + \ln\left(1 + e^{-\frac{3\beta\gamma}{L^2}} + \ldots\right) \approx -\frac{\beta\gamma}{L^2} + e^{-\frac{3\beta\gamma}{L^2}} + \ldots$$

where we used the approximation $\ln(1 + \epsilon) \approx \epsilon$.

(c) These quantities are given by (see lecture notes, note that here L plays the role of the volume V)

$$E = -\left(\frac{\partial \ln Z}{\partial \beta}\right)_L, \quad C = \beta^2\left(\frac{\partial^2 \ln Z}{\partial \beta^2}\right)_L, \quad P = \frac{1}{\beta}\left(\frac{\partial \ln Z}{\partial L}\right)_\beta.$$

Inserting the partition sum we obtain

$$E = \frac{\gamma}{L^2}\left(1 + 3e^{-\frac{3\beta\gamma}{L^2}} + \ldots\right), \quad C = \frac{9\beta^2\gamma^2}{L^4}e^{-\frac{3\beta\gamma}{L^2}}, \quad P = \frac{2\gamma}{L^3}\left(1 + 3e^{-\frac{3\beta\gamma}{L^2}} + \ldots\right)$$

(d) We are dealing here with a quantum-mechanical particle. Such a particle has a non-vanishing ground state energy. Changing the volume (the length L) at zero temperature will also change the value of the ground state energy. This means that work has to be done when compressing the system which manifests itself as a nonzero pressure even at zero temperature.

(e) In the limit $T \to \infty$ ($\beta \to 0$) the summands in the partition sum $Z(\beta, L) = \sum_{n=1}^{\infty} e^{-\frac{\beta\gamma n^2}{L^2}}$ vary only slowly with n so that we can approximate the partition sum by a continuous integral as follows. Setting $\Delta x = \sqrt{\beta\gamma}/L$ we rewrite

$$Z(\beta, L) = \sum_{n=1}^{\infty} e^{-\frac{\beta\gamma n^2}{L^2}} = \frac{1}{\Delta x} \sum_{n=1}^{\infty} \Delta x \, e^{-(n\,\Delta x)^2} \approx \frac{L}{\sqrt{\beta\gamma}} \int_0^{\infty} \mathrm{d}x \, e^{-x^2} = \frac{L}{\hbar} \sqrt{\frac{m}{2\pi\beta}} \,.$$

(f) The results read

$$E = \frac{1}{2\beta}\,, \quad C = \frac{1}{2}\,, \quad P = \frac{1}{L\beta}.$$

(Σ = 12P)