Q1. Consider a crystal of $N$ atoms in an external magnetic field $B$, where each atom can have one of three possible spin states $s_i \in \{-1, 0, +1\}$. The energy of an atom due to the external field is given by $\epsilon_i = -\mu Bs_i$, where $\mu$ is the unit magnetic moment. The crystal is kept at constant temperature $\tau = k_B T$.

(a) Ignoring other contributions to the energy, write down the partition function for the crystal.

(b) Calculate the internal energy of the crystal as a function of $\tau$. What is the internal energy in the limit $\tau \to \infty$?

(c) Find the heat capacity of the crystal and plot it as a function of $\tau$.

SOLUTION:

(a) The partition function for a single atom is

$$Z_1 = e^{\mu B / \tau} + 1 + e^{-\mu B / \tau} = 1 + 2 \cosh(\mu B / \tau)$$

and for $N$ atoms we have

$$Z_N = Z_1^N = \left[1 + 2 \cosh(\mu B / \tau)\right]^N.$$  

Note that we do not need a $(1/N!)$ in front of $Z_N$, since the atoms are fixed to their positions in the crystal.

(b) The internal energy is given by

$$U = -\frac{\partial \log Z_N}{\partial (1/\tau)} = -N\mu B \frac{2 \sinh(\mu B / \tau)}{1 + 2 \cosh(\mu B / \tau)}.$$

$$\lim_{x \to 0} \sinh(x) \to 0,$$ therefore $\lim_{\tau \to \infty} U(\tau) = 0$. This is obvious by the fact that at infinite temperature, all states are equally probable, i.e., the internal energy is the average of $+\mu B$, 0 and $-\mu B$.

(c) $C_V = \left. \frac{\partial U}{\partial \tau} \right|_V = N \left( \frac{\mu B}{\tau} \right)^2 \frac{2 + \cosh(\mu B / \tau)}{1 + 2 \cosh(\mu B / \tau)^2}$.

In the two extremes, we get:

$$C \simeq \begin{cases} \frac{N}{2} \left( \frac{\mu B}{\tau} \right)^2 & \text{for } \mu B / \tau \gg 1 \\ \frac{N}{2} \left( \frac{\mu B}{\tau} \right)^2 e^{-\mu B / \tau} & \text{for } \mu B / \tau \ll 1 \end{cases}$$
Q2. Consider the system in Problem 1, but now isolated at constant energy $E = +N\mu B/2$. In other words, $N_+ - N_- = N/2$ and $N_+ + N_0 + N_- = N$ where $N_+, N_0$ and $N_-$ are the number of atoms with spin $+1,0,-1$, respectively.

(a) What is the maximum and minimum possible $N_0$ at this value of the energy?

(b) For given $N_0$ what are the values of $N_+$ and $N_-$ at this energy?

(c) Express the entropy of this system as a function of a sum $\sum_{N_0=0} g_N(N_0)$.

(d) Calculate the typical number of spin-zero atoms $N_0$ by setting $\frac{d[\log g_N(N_0)]}{dN_0} = 0$.

(e) If you bring this system in contact with a heat reservoir at a temperature $T > 0$, which way do you expect the energy to flow? (no calculations necessary!)

SOLUTION:

(a) The given system has fixed particle number $N$ and energy $E = +N\mu B/2$. Using the two conditions $N_+ + N_0 + N_- = N$ and $N_+ - N_- = N/2$, we find $N_0 = N/2 - 2N_+$. Then, $N_0^{max} = N/2$, when $N_+ = 0$ and $N_- = N/2$.

(b) From above, $N_+ = N/2 - N_0$ and $N_- = 3N/2 - N_0$.

(c) For a fixed $N_0$, the number of ways $N_0$, $N_+$ and $N_-$ atoms can be chosen out of $N$ atoms is

$$g_N(N_0) \equiv \binom{N}{N_0} \binom{N-N_0}{N_-} = \frac{N!}{N_0!N_+!N_-!}.$$

The total number of microscopic states at fixed $(N, E)$ is the sum of $g_N(N_0)$ over the allowed values of $N_0$ calculated in part (a). Then the entropy is

$$\sigma(N, E) = \log \sum_{N_0=0}^{N/2} g_N(N_0) = \log \left[ \sum_{N_0=0}^{N/2} \frac{N!}{N_0!(N_0)^2!(\frac{3N}{4} - N_0)!} \right].$$

(d) For large $N$, the largest term in the sum dominates the system and determines the typical value of $N_0$. Maximum of $g_N(N_0)$ is also the maximum of $\log[g_N(N_0)]$, therefore we set $\frac{d}{dN_0} \log[g_N(N_0)] = 0$. Using Stirling’s approximation $\log N! \simeq N \log N - N$, we obtain

$$\left. 0 = \frac{d}{dN_0} \left[ N \log N - N + N_0 \log N_0 - N_0 + N_+ \log N_+ - N_+ + N_- \log N_- - N_- \right] \right|_{N_0} \right. = - \log N_0 + \frac{1}{2} \log \left[ \frac{N}{4} - \frac{N_0}{2} \right] + \frac{1}{2} \log \left[ \frac{3N}{4} - \frac{N_0}{2} \right].$$

Exponentiating both sides,

$$N_0^2 = \left( \frac{N}{4} - \frac{N_0}{2} \right) \left( \frac{3N}{4} - \frac{N_0}{2} \right) = \frac{N_0^2}{4} - \frac{N_0N}{2} + \frac{3N^2}{16}.$$

Solving the quadratic equation yields $N_0 = (\sqrt{13} - 2)/6N$.

(e) The energy of the system is larger than the value expected at infinite temperature (Problem 1), in other words, the system has negative temperature. Therefore the flow of energy will always be from the system to the reservoir.
Q3. We will investigate a single particle in a box of size $L \times L \times L$ in a gravitational potential. The Hamiltonian (energy) of the particle is given by

$$H = \frac{(p_x^2 + p_y^2 + p_z^2)}{2m} + mgz$$

where $m$ is the mass of the particle and $g$ is the gravitational acceleration.

(a) Calculate the partition function for a free particle first ($g = 0$) starting from

$$Z = \int \frac{dx \, dy \, dz \, dp_x \, dp_y \, dp_z}{h^3} \exp\left[-\frac{H_{\text{free}}}{\tau}\right]$$

and evaluating each integral within proper limits. Observe that with the proper factor $h^3$ you obtain $Z = V/\lambda^3$ as we obtained before.

(b) How is your answer modified for $g \neq 0$?

(c) Find the internal energy of the particle.

(d) Calculate the average height $\langle z \rangle$ of the particle (measured from the bottom of the box) when $L \gg \tau/mg$, by expressing it as a suitable derivative of the partition function.

SOLUTION:

(a) For $g = 0$, we find $H_{\text{free}} = (p_x^2 + p_y^2 + p_z^2)/2m$. In order to calculate $Z$, note that

$$\int_0^L dx = \int_0^L dy = \int_0^L dz = L$$

$$\int_{-\infty}^{\infty} \frac{dp_x}{h} e^{-p_x^2/2m\tau} = \int_{-\infty}^{\infty} \frac{dp_y}{h} e^{-p_y^2/2m\tau} = \int_{-\infty}^{\infty} \frac{dp_z}{h} e^{-p_z^2/2m\tau} = \frac{\sqrt{2\pi m\tau}}{h} = 1/\lambda$$

Then $Z_{\text{free}} = V/\lambda^3$, as expected.

(b) For $g \neq 0$ only the integral over $z$ will change. Instead of a factor of $L$, now it yields

$$\int_0^L dz \, e^{-mgz/\tau} = \frac{\tau}{mg} \left[1 - e^{-mgL/\tau}\right] \Rightarrow Z = Z_{\text{free}} \times \frac{\tau}{mgL} \left[1 - e^{-mgL/\tau}\right].$$

(c) The internal energy is

$$U = -\left. \frac{\partial \log Z}{\partial (1/\tau)} \right|_{V} = U_{\text{free}} - \left. \frac{\partial}{\partial (1/\tau)} \left( \log \left[ \frac{\tau}{mgL} \left(1 - e^{-mgL/\tau}\right) \right]\right) \right|_{V}$$

$$= 3 \frac{2}{2^\tau} + \frac{mgL}{e^{mgL/\tau} - 1} = \frac{5}{2} \tau - \frac{mgL}{e^{mgL/\tau} - 1}.$$

(d) By inspection,

$$\langle z \rangle = \left. -\tau \frac{\partial \log Z}{\partial (mg)} \right|_{V,\tau} = \frac{\tau}{mg} - \frac{L}{e^{mgL/\tau} - 1}.$$

It also follows from part (c) after expressing the internal energy as

$$U = \langle |\vec{p}|^2/2m \rangle + mg\langle z \rangle = 3\tau/2 + mg\langle z \rangle.$$