1. (18 points) Consider a spin $1/2$ particle with magnetic moment $\mu$ placed in a magnetic field $H_0$ at temperature $T_0$. The temperature $T_0$ is chosen such that the state of energy $-\mu H_0$ is twice as probable as that of energy $+\mu H_0$. Since these two probabilities have to add up to one, that means that the probability for a particle to be in a state with energy $-\mu H_0$ is equal to $2/3$, while that for being in the state with energy $+\mu H_0$ is $1/3$.

(a) (3 points) Show that $e^{\beta_0 \mu H_0} = \sqrt{2}$, with $\beta_0 = 1/(kT_0)$. Calculate the average energy per particle.

(b) (3 points) The field strength is increased quasistatically from $H_0$ to $2H_0$, while the temperature is held constant at $T_0$. Show that the probabilities for the two states become $4/5$ and $1/5$, respectively. Calculate the average energy per particle for the new field strength.

(c) (4 points) Starting from the original situation, the temperature is decreased quasistatically from $T_0$ to $T_0/2$, while the field is held constant at $H_0$. Calculate the probabilities for the two states, and the average energy per particle.

(d) (4 points) Now the field strength is increased *adiabatically* and quasistatically from $H_0$ to $2H_0$. What are the probabilities for the two states after this change? Calculate the average energy per particle.

(e) (4 points) For cases (c) and (d), indicate whether the heat absorbed by the system and the work done by the system are positive, negative, or zero.

2. (16 points) For a non-interacting Bose–Einstein gas (in three dimensions, and non-relativistic), we have (using the grand-canonical ensemble),

$$\frac{PV}{kT} = \log Z_G = - \sum_s \log \left( 1 - e^{-\beta (\epsilon_s - \mu)} \right),$$

where the sum is over all single-particle states $s$, with single-particle energies $\epsilon_s$. In this equation $\beta = 1/(kT)$, with $T$ the temperature, $\mu$ is the chemical potential, $P$ the average pressure, and $V$ the volume. The average number of particles in state $s$ is

$$\bar{n}_s = \frac{1}{e^{\beta (\epsilon_s - \mu)} - 1}.$$
(a) (5 points) Show that the entropy $S$ is given by

$$S = k \sum_s [(1 + \bar{n}_s) \log (1 + \bar{n}_s) - \bar{n}_s \log \bar{n}_s].$$

(b) (5 points) Show that, for the Bose–Einstein gas

$$\lim_{T \to 0} S = 0.$$

(c) (6 points) Derive a similar formula for the entropy of a non-interacting Fermi–Dirac gas, and show again that $S = 0$ at $T = 0$.

3. (16 points) In this problem we will consider a copper (Cu) and zinc (Zn) alloy. This alloy has a crystal structure in which the atoms are located on the sites of a body-centered cubic (bcc) lattice. A bcc lattice consists of a simple cubic lattice, with an extra lattice site at the center of each simple cube. We will refer to the simple cubic lattice as “sub-lattice 1.” The sites at the centers form a simple cubic lattice themselves, which we will refer to as “sub-lattice 2.” At $T = 0$, the Cu atoms are located on the simple cubic lattice, i.e. on sub-lattice 1, and the Zn atoms are located on the sites at the centers of the simple cubes, i.e. on sub-lattice 2. All of the sites are always occupied by either a Cu or a Zn atom. At temperatures larger than zero, the atoms may move around, so one may have a Zn atom on sub-lattice 1, and Cu atoms may happen to be sub-lattice 2. We will assume that the internal energy of a configuration of Cu and Zn atoms only gets contributions from nearest-neighbor pairs of sites (note that the nearest neighbor of a corner site is a center site and vice versa). The contribution of a nearest-neighbor pair is $e_{CC}$ if both are occupied by Cu atoms, $e_{ZZ}$ if both are occupied by Zn atoms, and $e_{CZ}$ if one is occupied by a Cu atom and one by a Zn atom. We will take the total number of lattice sites $N$ to be large, and we will ignore any boundary effects. Since there are equally many corner and center sites, we will assume that the total number of Cu atoms is equal to the total number of Zn atoms.

(a) (6 points) Let $n_{iC} = 1$ if a Cu atom occupies site $i$, and $n_{iC} = 0$ if not. Likewise, let $n_{iZ} = 1$ if a Zn atom occupies site $i$, and $n_{iZ} = 0$ if not. It follows that, for each site $i$, $n_{iC} + n_{iZ} = 1$. We may write

$$n_{iC} = (1 + \sigma_i)/2,$$

$$n_{iZ} = (1 - \sigma_i)/2,$$

with $\sigma_i = \pm 1$. Show that the internal energy of a configuration of Cu and Zn atoms can be written as

$$E = \sum_{\langle ij \rangle} \left[ \frac{1}{4} (e_{CC} + e_{ZZ} - 2e_{CZ}) \sigma_i \sigma_j + \text{constant} \right],$$

where $\sum_{\langle ij \rangle}$ denotes the sum over all nearest-neighbor pairs. Give the details of your argument leading to this expression for $E$.

(b) (4 points) Given what we know about the crystal at $T = 0$, argue that $J = \frac{1}{4} (e_{CC} + e_{ZZ} - 2e_{CZ}) > 0$. Explain your reasoning precisely.
(c) (6 points) The energy $E$ we found in part (a) looks like that of the ferromagnetic Ising model, except that the sign of $J$ is opposite, so $E$ is the energy of the anti-ferromagnetic Ising model. In order to make it look like the ferromagnetic Ising model, we perform a transformation on the variables $\sigma_i$, introducing new variables $\tau_i$, which like the $\sigma_i$ also take the values $\pm 1$, such that the energy expressed in terms of the $\tau_i$ is

$$E = -J \sum_{\langle ij \rangle} \tau_i \tau_j,$$

up to an additive constant. Find this transformation, i.e., express the $\tau_i$ in terms of $\sigma_i$. We know that this ferromagnetic Ising model undergoes a phase transition, with $\langle \tau_i \rangle \neq 0$ for $T < T_c$, and $\langle \tau_i \rangle = 0$ for $T > T_c$, with $T_c$ the critical temperature. Argue that this implies that for $T > T_c$ there are on average equally many Cu atoms on sub-lattice 1 as on sub-lattice 2 (and thus the same thing is true for Zn atoms), while for $T < T_c$ there are more Cu atoms on sub-lattice 1 than on sub-lattice 2.