Problem Sheet 3 (Chapter 8 (and a bit of 7))

1. This question is about thermodynamic stability (Sec. 7.g). Consider a hypothetical system described by the *equation of state*

$$S = cU^p,$$

where $c \geq 0$ and p are constants, and we can assume $U \geq 0$.

   (a) Find $T(U)$, the system's temperature as a function of energy.

   (b) Hence find $S(T)$, and the heat capacity $C = T\frac{\partial}{\partial T}S$.

   (c) For what values of p is the system thermodynamically stable?

2. This question relates to the virial coefficient in Sec. 8b.

   (a) Evaluate $B_2(T)$ for the case of a "hard-sphere" model of interactions where $U(r) = 0$ for $r > 2a$, and $U(r) = +\infty$ for $r \leq 2a$. Here a is the radius of the "hard sphere" which models each molecule.

   (b) Hence evaluate Eq. (8b.5), and rewrite it as $PV' = Nk_BT$, for

$$V' = V - \frac{1}{2} \times N \times \frac{4}{3}\pi(2a)^3.$$

   Interpret the three factors being multiplied in the second term. (The $\frac{1}{2}$ is probably the trickiest to interpret.)

3. This question relates to the 1D Ising model.

   (a) Derive yourself the characteristic equation in Eq. (8.h4). Are the eigenvalues always real? Are they always positive?

   (b) Derive Eq. (8h.7), using the method in the notes.

   (c) Derive the full expression for $\langle s_1 s_{1+r} \rangle$ for arbitrary r. What is interesting about it for $J < 0$?

(d) Using this type of approach, rederive Eq. (8h.7) as $\langle s_1 \rangle$.

4. This question relates to the mean-field model of ferromagnetism for the case of no applied field ($B = 0$). In the notes, we showed graphically that there are two self-consistent mean-field with a spontaneous mean-field $\bar{B} \neq 0$. But there is also a solution with $\bar{B} = 0$, which we ignored for no good reason. Here we rectify that by using a more sophisticated theory.

   (a) Derive an expression for $S_1(\bar{s})$, the entropy of single spin-half particle, in a mixture of being spin up ($s = +1$) and spin down ($s = -1$), as a function of its mean spin $\bar{s}$. Hence derive an expression for $S_N(\bar{s})$, under the mean-field approximation where each spin is independent.

   (b) Now consider the energy of spin n. In the mean field approximation, this is given by $U_1 = -\alpha \bar{B} \bar{s}_n$, and $\bar{B}$ is a result of a large number of other spins: $\alpha \bar{B} = \sum_{p \neq n} J(|p-n|) s_p$. Thus, ignoring correlations between spins,

$$U_1 = -\bar{s}_n \sum_{p \neq n} J(|p-n|) \bar{s}_p.$$

   For a model with periodic boundary conditions, where all spins are equivalent, we can assume $\bar{s}$ is the same for all spins. This would seem to imply a total energy

$$U_N = -\sum_n \bar{s} \sum_{p \neq n} J(|p-n|) \bar{s} = -GN\bar{s}^2,$$

   where $G = \sum_{p \neq n} J(|p-n|)$ as in the notes. The problem is that more fundamentally this corresponds to setting the total Hamiltonian as

$$\hat{H} = -\sum_n \sum_{p \neq n} J(|p-n|) \hat{s}_n \hat{s}_p,$$

   which counts every interaction term twice. That is, we would get a term $J(2)\hat{s}_1\hat{s}_3$ from $n = 1$ and $p = 3$, plus a term $J(2)\hat{s}_3\hat{s}_1$ from $n = 3$ and $p = 1$. The correct total Hamiltonian is

$$\hat{H} = -\tfrac{1}{2} \sum_n \sum_{p \neq n} J(|p-n|) \hat{s}_n \hat{s}_p.$$

(Recall a similar argument in Sec. 4.3.1 of the QED notes.) Thus the correct total energy in the mean-field approximation is

$$U_N = -\tfrac{1}{2}\sum_n \bar{s} \sum_{p\neq n} J(|p-n|)\bar{s} = -\tfrac{1}{2}GN\bar{s}^2,$$

Hence — and this is where we finally get to the question — write down an expression for the total *free energy*, as a function of $\bar{s}$.

(c) Show that the mean-field states (described by $\bar{s}$) which minimize free energy correspond exactly to the non-zero mean-field solutions found in the notes, when $T < T_\mathrm{C}$. What happens when $T = T_\mathrm{C}$? $T > T_\mathrm{C}$?

You may find the following site helpful:
www.desmos.com/calculator/1fu7ffukkd

5. This question also relates to the mean-field model of ferromagnetism. Using this theory, estimate the Curie temperature T_C of a face-centred cubic (see figure) spin-1/2 Ising ferromagnet with a ferromagnetic nearest-neighbour coupling constant J_{np} = .03eV and an antiferromagnetic next-to-nearest-neighbour coupling constant of magnitude 0.02eV. Ignore more distant neighbour couplings.