Answer THREE questions.

The numbers in square brackets at the right-hand margin indicate the provisional allocation of marks per sub-section of a question.

You may assume the following values:

Electronic charge $e = 1.60 \times 10^{-19}\,\mathrm{C}$; $1\,e\mathrm{V} = 1.60 \times 10^{-19}\,\mathrm{J}$

Boltzmann constant $k_B = 1.38 \times 10^{-23}\,\mathrm{J\,K^{-1}}$

Muon lifetime $= 2.2\,\mu\mathrm{s}$

Muon gyromagnetic ratio $\gamma_\mu = 2\pi \times 136\,\mathrm{kHz\,(mT)^{-1}}$

Nuclear magneton $\mu_N = 5 \times 10^{-27}\,\mathrm{A\,m^{-2}}$

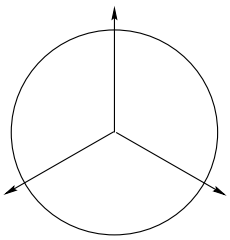
Magnetic dipole moment of Cu nucleus $\mu_{\mathrm{Cu}} = 2.6\mu_N$

Permeability of free space $\mu_0 = 4\pi \times 10^{-7}\,\mathrm{H\,m^{-1}}$

Lattice constant of fcc Cu $= 0.36\,\mathrm{nm}$; Cu-Cu interatomic distance $= 0.26\,\mathrm{nm}$

Ratio of muon to proton masses $m_\mu/m_P = 1/9$

1. (a) *Flatland* is a two-dimensional world. In Flatland, molecules of the substance Mercedium possess an attractive part to their intermolecular potential that has trigonal symmetry, with each molecule being attracted to others through 'arms' disposed at 120° to each other (see diagram). The individual molecules are prevented from overlapping by a soft *spherically symmetrical* repulsive core characterised by a van der Waals type radius r_0



(i) At low temperature T and pressure p, Mercedium has a crystalline phase. Sketch the structure you would expect this phase to have, and calculate its packing density when neighbouring molecules are in contact a distance $2r_0$ apart. **[3]**

(ii) Assuming a liquid phase exists when the crystal is heated sufficiently, sketch the (p, T) section of the phase diagram you expect Mercedium to have. Explain why this phase diagram differs from that you would expect from a substance in which the attractive part of the potential is spherically symmetrical (like a two dimensional van der Waals system). **[4]**

(iii) Referring to your phase diagram, describe and explain what you would expect to happen when you increase pressure isothermally on a crystal of Mercedium initially at a (p, T) point just below the melting line. **[2]**

(iv) A crystalline sample of Mercedium is heated to form the liquid at a temperature just above its melting point. This sample is now further heated slowly. With the aid of a sketch of density against temperature, discuss how you think the density will vary with temperature, explaining your reasoning. **[3]**

(b) In our world of three spatial dimensions, water is thought to be crucial in e.g. maintaining climatic stability and facilitating life processes. Although we do not understand fully the role of water in such processes, it is generally believed that the structural versatility of the water molecule that is a consequence of its ability to both *donate two and accept two hydrogen bonds* in an approximately *tetrahedral geometry* is of significant importance.

Bearing in mind these characteristics of three dimensional water, discuss with reasons the extent to which you think that a water-like material could or could not exist in Flatland. Comment on aspects of your candidate two dimensional water molecules that you think might be important in your discussion. **[8]**

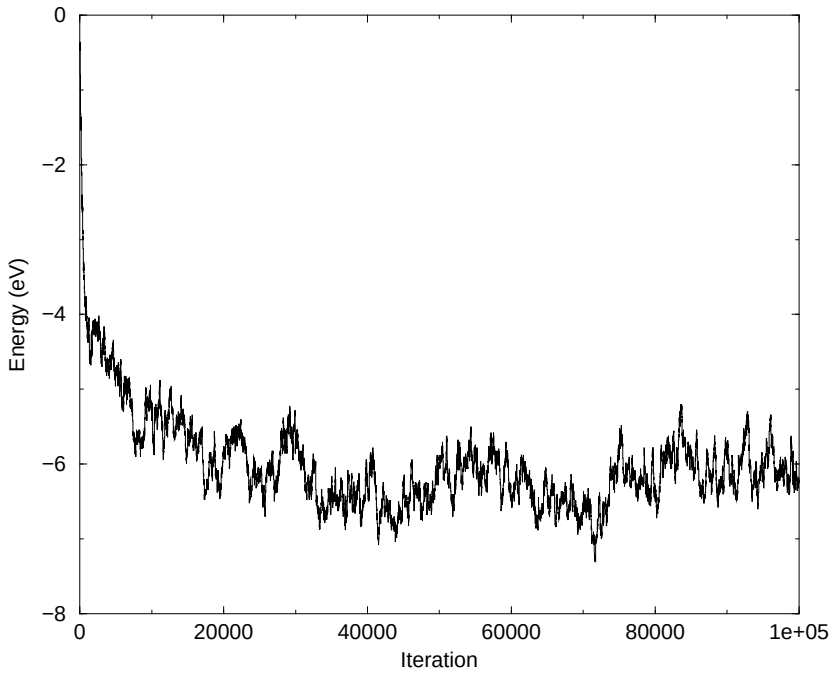
2. (a) Outline the principles of the Monte Carlo technique for simulations of material properties. **[4]**

Explain what it means to say that a Monte Carlo algorithm is (i) 'Markovian' and (ii) 'stationary', and explain what the requirement of 'detailed balance' in a stationary Markovian Monte Carlo algorithm means. Show that the distribution of states sampled by a stationary Markovian Monte Carlo procedure can converge to the thermal equilibrium distribution only if the detailed balance condition is satisfied. **[5]**

In a particular Monte Carlo algorithm, the probability of accepting a move from an initial configuration r to a new trial configuration r' (randomly generated in a manner that does not discriminate between forward and reverse moves) is

$$\frac{\exp[-(E_{r'} - E_r)/2k_BT]}{2\cosh[(E_{r'} - E_r)/2k_BT]},$$

where E_r and $E_{r'}$ are the energies of the configurations. Show that this algorithm satisfies the detailed balance condition. **[3]**



(b) The figure shows the energy in a certain Monte Carlo simulation as a function of the iteration count. The temperature is $T = 300\,\mathrm{K}$.

(i) How many iterations do you think are needed before the system is equilibrated? **[2]**

(ii) Approximately how often could statistically independent samples of the energy of this system be taken? **[2]**

(iii) From the data, make an approximate estimate the heat capacity of the system being simulated. **[4]**

3. Explain the principles of the technique of low-energy electron diffraction (LEED). Your answer should include a discussion of the conservation laws involved in the scattering, and a diagram showing the allowed scattering directions. Why is the technique surface-sensitive? **[5]**

Draw a diagram illustrating the structure of the unreconstructed (001) surface of silicon and explain why this structure for the surface is unstable. What is the nature of the (2×1) reconstruction that occurs on this surface, and why does it lower the surface energy? What effect does the reconstruction have on the electronic properties of the clean surface? **[5]**

Show in a sketch how the LEED patterns of the unreconstructed surface and of a single-domain (2×1) reconstruction would differ. How would the presence of monolayer steps on the surface affect the LEED patterns? **[3]**

Explain what is observed in scanning tunnelling microscopy (STM) of the Si(001) surface (i) at room temperature; (ii) at low temperature. Explain why the images differ, and interpret them in terms of a model of the atomic-scale surface structure. **[4]**

How would the LEED pattern of the low-temperature surface differ from that of the room-temperature surface? **[3]**

4. (a) The result of a single neutron scattering experiment on a hydrogenous liquid system can be written as:

$$F_H(Q) = c_H^2 b_H^2 (S_{HH}(Q) - 1) + 2 c_H b_H c_X b_X (S_{XH}(Q) - 1) + c_X^2 b_X^2 (S_{XX}(Q) - 1) \quad (1)$$

where c_H and c_X represent the fractions of hydrogen and non-hydrogen atomic sites respectively, b_H and b_X the hydrogen atom and non-hydrogen atom scattering lengths whilst $S_{HH}(Q)$, $S_{XH}(Q)$ and $S_{XX}(Q)$ are the partial structure factors corresponding respectively to the interatomic pair correlations between hydrogen sites themselves, between hydrogen sites and non-hydrogen atomic sites and finally between non-hydrogen sites themselves.

(i) What structural information could you obtain on this system if you performed also a second experiment in which all the hydrogen atoms were replaced by deuterium? **[4]**

(ii) By performing an appropriate third experiment, it is possible to determine the partial structure factor $S_{HH}(Q)$. What sample would you use for this third experiment and why? **[4]**

(iii) Write down the three equations similar in form to equation 1 that describe this three sample experiment, defining any new term or terms that you introduce. **[2]**

(iv) An assumption you need to make is that the structure of a hydrogenous liquid system is to first order independent of its isotopic composition. Suggest how this assumption could be tested experimentally. **[3]**

(b) In the figure are shown (top) the three partial distribution functions that correspond to the inter-atomic pair distributions of oxygen and hydrogen atoms in liquid water. Also shown (bottom) are a schematic diagram of a water molecule and a typical configuration of such molecules that may be expected in the liquid state. Using the information provided in the figure, estimate:

(i) The $H - O - H$ angle on an individual water molecule; **[2]**

(ii) The $O_1 - O_3 - O_5$ angle that is characteristic of the illustrated molecular configuration. **[2]**

Finally, from an inspection of the pair distribution functions, what can be said about the linearity of the $O - H \ldots O$ intermolecular hydrogen bond that exists in liquid water? **[3]**

5. Discuss the use of implanted positive muons (i) as magnetic probes, e.g. in magnetic or superconducting material, and (ii) as proton substitutes. **[6]**

The figure shows a μSR histogram (left) and asymmetry signal (right) for muons in copper metal. Referring to the figure, and using information at the head of the paper, answer the following:

(a) Sketch a typical arrangement of muon beam, sample, and positron detectors used to obtain data such as these. The time channels or "bins" have width 16ns. If there are 10^6 total counts in the histogram (left part of figure), how many are there in (i) the 1^{st} and (ii) the 500^{th} bin? **[3]**

(b) What is the cause of the asymmetry in the muon decay? Why does the noise increase with elapsed time in the asymmetry plot (right part of figure) and how may this be decreased? **[2]**

(c) What magnetic field was used in this experiment? **[1]**

(d) The damping of the asymmetry signal is due to the dipolar fields from Cu nuclei adding to and subtracting from the applied field. Estimate these local fields from the damping. Show that they are compatible with Cu nuclear moments about 0.2nm away from the interstitial muon. What distance would you expect between an interstitial muon and neighbouring Cu nuclei in the fcc copper lattice? **[5]**

What would happen to the damping rate when the muons start to diffuse? What differences might there be between the diffusion mechanism for muons and protons? How do the zero-point energies for the two particles compare within the same potential well? **[3]**

[You may ignore angular variations and assume that the dipolar field of a Cu nucleus behaves as a function of distance like

$$B_{\text{dip}} \sim \frac{\mu_{\text{Cu}}\mu_0}{4\pi r^3},$$

where μ_{Cu} is the nuclear magnetic moment of Cu.]