Sheffield Hallam University

Department of Engineering and Mathematics

Session:	2018/19
Module:	55-402182 Introduction to Condensed Matter Physics
Module Leader:	Simon Clark
Assignment number/title:	Assignment 3
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Maximum word count or number of pages:	N/A
Percentage contribution to overall module mark:	30%
Deadline for submission:	3pm Thurs 25$^{\text{th}}$ April 2019
Method and Location for Submission:	Online Submission
Deadline for return of feedback:	Friday 17$^{\text{th}}$ May 2019

Module learning outcomes to be assessed:

- Conduct individually investigations and analysis related to applications of condensed matter physics.

References/recommended reading:

See Library Reading Lists Online.

Please ensure that all sources of information used are referenced. For guidance see http://libguides.shu.ac.uk/referencing

This is an individual assignment.

All assessments are subject to SHU's collusion and plaigiarism regulations. Please refer to: https://students.shu.ac.uk/shuspacecontent/assessment/plagiarism

Please submit your work working out and Python program as separate files via Blackboard.

Any hand written work should be scanned and submitted electronically via Blackboard.

In this assignment, you will be determining the temperature dependence of magnetisation in a ferromagnetic material based on mean field theory. A ferromagnetic material has a spontaneous magnetisation (think a bar magnet - it keeps its magnetic field) that depends on temperature. The origin of this magnetism can be thought of as being due to many small magnets (magnetic moments) that reside on each atomic site. The magnetic moments will preferentially remain aligned due to (what can be thought of as) a kind of "force" known as the exchange interaction. To completely understand the origin of the exchange interaction, you need quantum mechanics, but for now we are just going to say that for each atom, there is an interaction with its nearest neighbours that makes them all want to stay aligned. This is shown schematically in panel a) of figure 1.

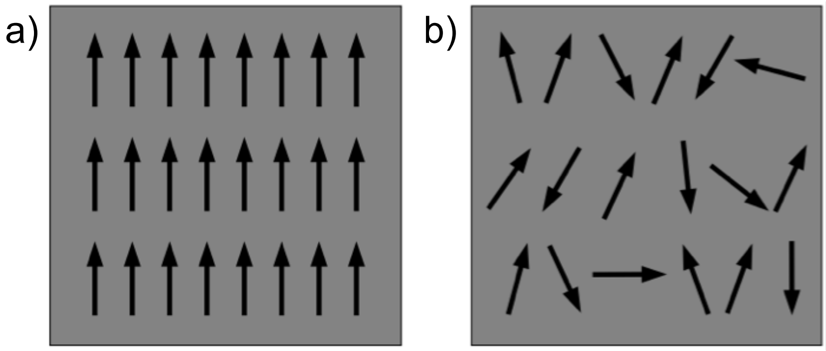

Figure 1: a) A schematic representation of magnetic moments on atomic sites aligned due to the exchange interaction in a ferromagnetic material. At 0K, without the presence of thermal fluctuations, the magnetic moments completely align, giving the maximum magnetization, known as the saturation magnetisation. b) Due to the presence of thermal fluctuations, the magnetic moments disorder and at the critical temperature the magnetisation goes to zero.

As well as the exchange interaction, at temperatures above zero Kelvin, there are thermal fluctuations that affect how the magnetic moments align. As the temperature increases, the thermal fluctuations become larger to such an extent that at some critical temperature, the magnetisation completely disappears. This temperature is known as the Curie temperature. This is sketched in panel b) of figure 1.

There are several theories that describe finite temperature magnetic properties, one such theory is the famous mean field (or Curie-Weiss) theory. The magnetisation can be related to the exchange interaction and an externally applied magnetic field, through the expression:

$$m = \tanh\left(\frac{\mu_0 \mu_{\mathrm{B}} H}{k_{\mathrm{B}} T} + \frac{zJm}{k_{\mathrm{B}} T}\right) \tag{1}$$

where, m is the magnetisation at a given temperature, T, divided by the saturation magnetisation at 0K (the saturation magnetisation), $m = M/M_0$. J is the exchange interaction constant between the nearest neighbours. The permeability of free space, $\mu_0 = 4\pi \times 10^{-7}$ TmA^{-1} and μ_{B} is the Bohr magneton, having a value of 9.27×10^{-24} J/T. H is an applied magnetic field with units of Am^{-1} and k_{B} is Boltzmann's constant with units of JK^{-1}.

Description of method

You will notice that this equation is not as straightforward to solve as it first appears, because the quantity, m, appears on both sides of the equation. This is known as a transcendental equation and we must solve it by what is known as a *self-consistent* approach. Obviously, for a given temperature, T, the solution to this equation is satisfied when the left hand side is equal to the right hand side. But how do we know when this is the case? One way is to imagine the left and right as separate functions, with the left hand side being simply a graph of $y = m$ and the right hand side being equal to $y = \tanh(\frac{\mu_0 \mu_B H}{k_B T} + \frac{zJm}{k_B T})$. This is shown graphically below on figure 2 (ignoring the applied field, so $H = 0$).

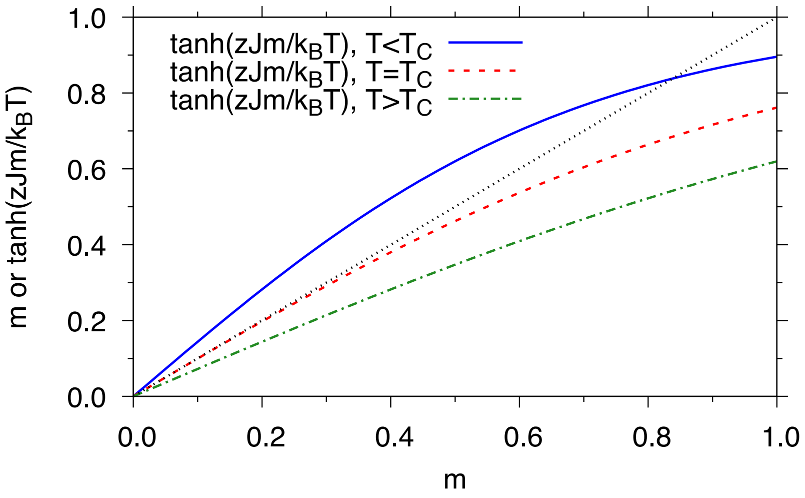

Figure 2: Graphical representations of the solutions to equation 1. The dotted black line represents $y = m$ (left hand side of equation 1), which does not change with temperature. The blue solid line represents the right hand side of equation 1 for $T < T_C$. The red dashed and green dot-dashed lines represent the case where $T = T_C$ and $T > T_C$, respectively. Notice that for all curves that there is a solution at $m = 0$, which is not a valid solution for $T < T_C$. Also, for $T = T_C$, the gradients of the two curves are equal at $m = 0$.

By finding where these curves cross for each temperature, one can find how the magnetisation varies with temperature, which is shown in figure 3.

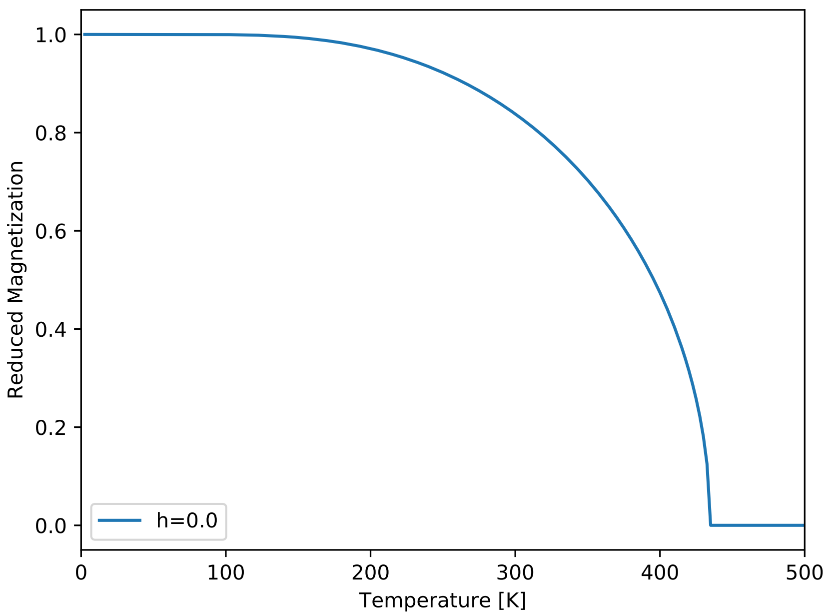

Figure 3: Numerical solutions to equation 1 giving the magnetisation as a function of temperature.

Algorithm

- For each temperature, vary m in small steps from 0 to 1.

- For each value of m, determine whether the values are equal (or close to being equal - recall the difficulties in comparing floating point numbers).
- Store the value of the crossing point as this will be the value of the equilibrium magnetisation at that temperature.
- Once this crossing point has been found, change temperature and find the new magnetisation.

There are several points to note about this algorithm:

- Starting at exactly T=0K often leads to errors as the two curves only cross at the origin.
- How you vary m will affect (i) the performance - too small and the program will take too long to run and (ii) the accuracy - if it is too large, then the estimate of the crossing point will be incorrect

Question 1

a) Write a python code to find the magnetisation as a function of temperature without the presence of an applied field for bcc Fe which has a value of $J = 1.8 \times 10^{-21}$ J and $z = 8$ nearest neighbours.

(50 marks)

b) Using the Matplotlib library, plot a fully labelled graph (including axis labels and a key) of your solution to part a) across a sensible range. You can test your code to part a) by noting that the relationship between the Curie temperature (when m goes to zero) and the exchange constant (see question 2) is given by equation 2. If you do not check your solution to part a) you will receive half marks for your plot. You must provide your code for this question in addition to the code for part 1b.

(10 marks)

Question 2

a) In the caption for figure 2, it is noted that at $T = T_C$ (without an applied field) the gradient (d/dm) of the left hand side and right hand side of equation 1 become equal at $m = 0$. Use this property to show, by hand, that the relationship between the Curie temperature and the exchange constant is given by:

$$k_{\mathrm{B}}T_{\mathrm{C}} = zJ \tag{2}$$

(10 marks)

b) Using your code from part 1a) find the magnetisation as a function of temperature for applied fields of $h = 0.0005$, 0.001 and 0.0015 and create a fully labelled plot of these curves along with your original curve for $h = 0$ on the same graph using Matplotlib. You should provide your code for this question in addition to the code for parts 1b and 1c. Note that $h = \mu_0\mu_{\mathrm{B}}H/k_{\mathrm{B}}T_{\mathrm{C}}$.

(25 marks)

c) What do you notice about the difference between the case where $h = 0$ and $h \neq 0$?

(5 marks)