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Solids 1 Test 3

1) **The simplest model for an ideal ferromagnet is called the Ising model. It is closely related to the Heisenberg model, except the Ising model spins are restricted to be either parallel or antiparallel. Assume that the** $S = \pm\frac{1}{2}$ **spins are oriented perpendicular to the plane of the array, and that the exchange strength** $J = 0.05eV$**.**

a) **Use the Monte Carlo method to do a computer simulation and determine the magnetization of a 10 by 10 square array of spins as a function of temperature. In the Monte Carlo simulation, assume that the probability of a spin flip is given by** $e^{-\frac{\Delta E}{kT}}$ **if the spin f lip would increase the energy, and equal to 1 if it decreases the energy. Explain the assumptions you make. Find the spontaneous magnetization** M **at** $T = 0K$ **and higher values up to the critical temperature** T_C**.**

I will write this program in Mathematica. In it, I have assumed periodic boundary conditions. The functions are as follows:

EnergyDiff—Given a sample, calculate the energetic change due to a flip.

DoCell—Use the algorithm described above to modify a cell.

MonteCarloEvolve—Run the Monte Carlo algorithm the specified number of times.

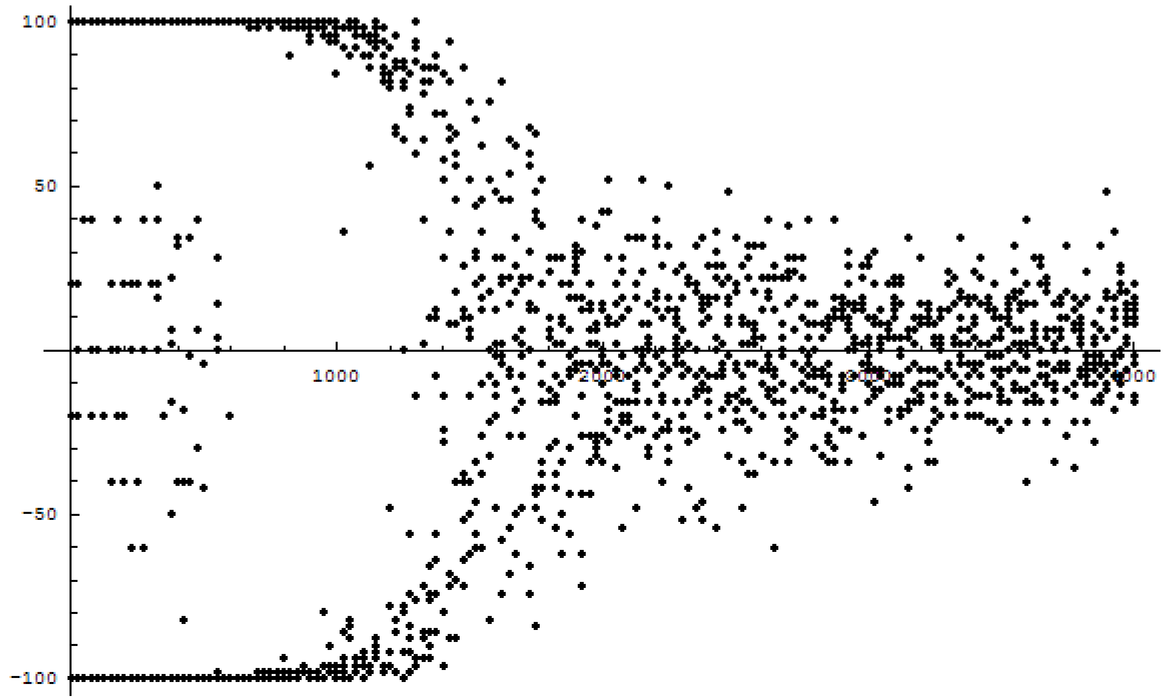
Magnetization—Calculate the magnetization in terms of “cells” for this sample.

AverageAbsoluteValMagnetization—Determine the average absolute magnetization for a number of trials.

AverageMagnetization—Determine the average magnetization for a number of trials.

```
EnergyDiff[Sample_, SizeX_, SizeY_, x_, y_] :=
  2
   (Exchange Sample[[x]][[y]]
      (Sample[[Previous[SizeX, x]]][[y]] + Sample[[Next[SizeX, x]]][[y]] +
        Sample[[x]][[Previous[SizeY, y]]] + Sample[[x]][[Next[SizeY, y]]]) +
     g uBohr Sample[[x]][[y]] BField);

DoCell[Sample_, SizeX_, SizeY_, x_, y_, T_] :=
  If[EnergyDiff[Sample, SizeX, SizeY, x, y] < 0, -1,
   If[Random[Real, {0, 1}, 5] < Exp[-EnergyDiff[Sample, SizeX, SizeY, x, y]/(k T)],
    -1, 1]];

MonteCarloEvolve[Sample_, SizeX_, SizeY_, Steps_, T_] :=
  Block[{workingSample = Sample},
   Do[ x = Random[Integer, {1, 10}]; y = Random[Integer, {1, 10}];
    Part[workingSample, x, y] *= DoCell[workingSample, SizeX, SizeY, x, y, T],
    {Steps}]; (workingSample )];

Magnetization[Sample_, SizeX_, SizeY_] :=
  Block[{total = 0}, For[x = 1, x ≤ SizeX, x++,
    For[y = 1, y ≤ SizeY, y++, total += Part[Sample, x, y] ]]; total];

AverageAbsoluteValMagnetization[SizeX_, SizeY_, T_, trials_, depth_] :=
  Block[{tempSample, total = 0},
   Do[tempSample = Table[If[Random[Integer] == 0, -1, 1], {SizeX}, {SizeY}];
    total += Abs[Magnetization[MonteCarloEvolve[tempSample, SizeX, SizeY, depth, T],
       SizeX, SizeY]], {trials}]; total / trials];

AverageMagnetization[SizeX_, SizeY_, T_, trials_, depth_] :=
  Block[{tempSample, total = 0},
   Do[tempSample = Table[If[Random[Integer] == 0, -1, 1], {SizeX}, {SizeY}];
    total += Magnetization[MonteCarloEvolve[tempSample, SizeX, SizeY, depth, T],
      SizeX, SizeY], {trials}]; total / trials];
```

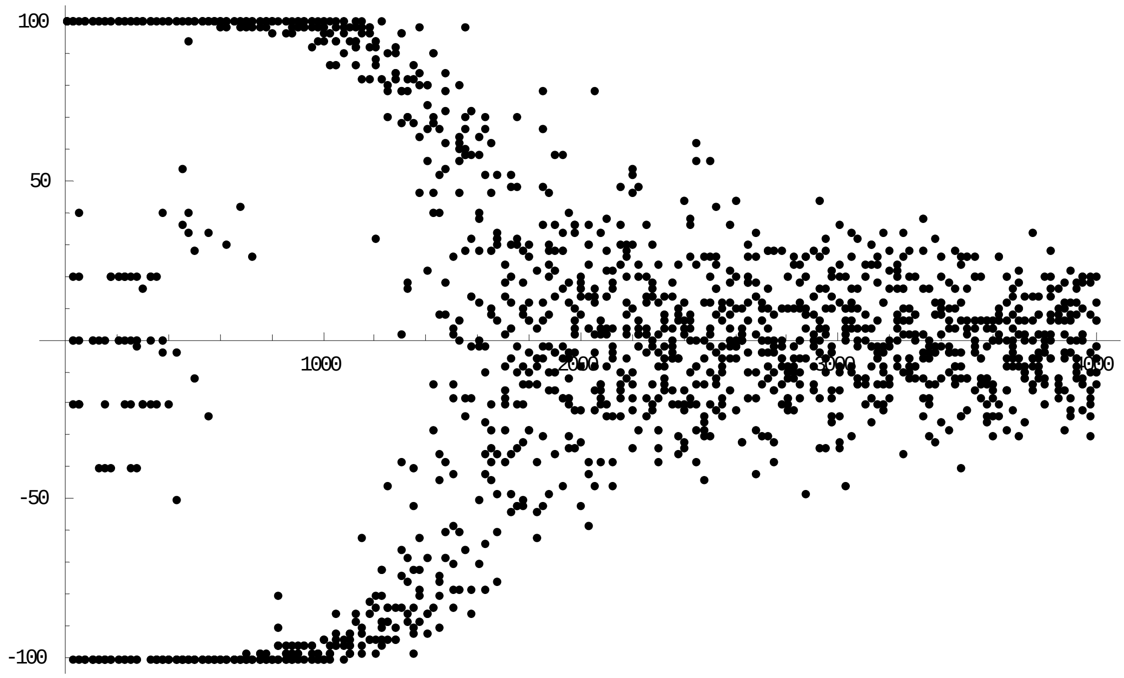
Running 10 samples for 25-Kelvin increments from 0.00001 Kelvin to 4000 Kelvin clearly shows the Curie temperature at roughly 1800K. The scale on the left-hand side represents the total magnetization of the sample, defined as the sum of the spins (count 1 as up, -1 as down). The magnetization at 0K should then correspond to [Insert MS Equation here: 2 g uB times 100].



b) **Repeat the simulations for the same array in a small magnetic field of $0.01T$, and plot $M(T)$. Assume the field is applied perpendicular to the plane and that the g-factor is free-electron-like. You can ignore the magnetostatic interactions between the different spins.**

The correction is then $\Delta E = g\mu_B sB$, where $s = \pm 1$ indicates spin-up or spin-down (the one-half appears in the Bohr magnetion $\mu_B = \frac{e\hbar}{2m}$. The free-electron g-factor is approximately 2.

Making these substitutions, it appears that this field has a very, very weak effect on the total magnetization on the material (in units of up spins minus down spins):



(Above: H = 0.01T, exchange interaction active)

(Above: H=0.01T, exchange interaction not active).

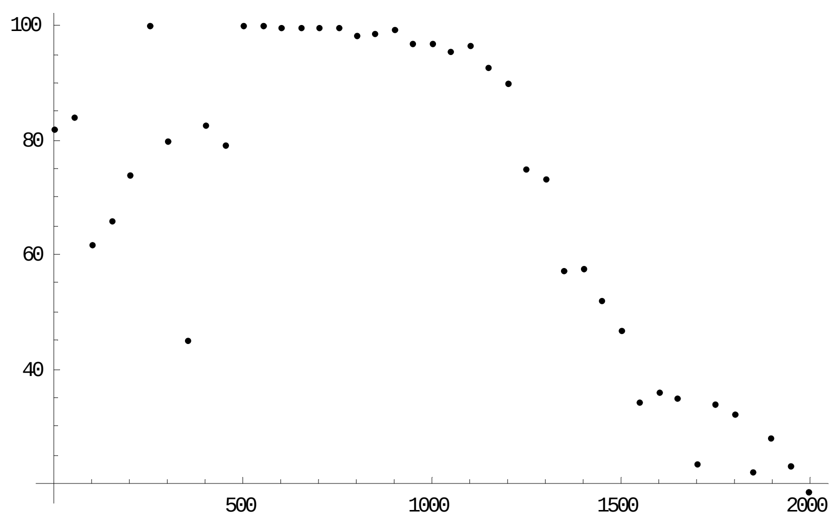
Experiments were run for 10000 Monte Carlo steps, with 10 samples per temperature. Averaging the magnetization for each temperature yields a seemingly random magnetization in each cases, indicating that either many more Monte Carlo steps should be used or that a sample much larger than 10 by 10 in order to capture a more accurate magnetization due to this field.

However, apparent from the top graph, it is clear that this field is much smaller than the field necessary to flip the spin of the magnet through saturation—apparently, the magnet is able to retain its opposing magnetization in the face of this field.

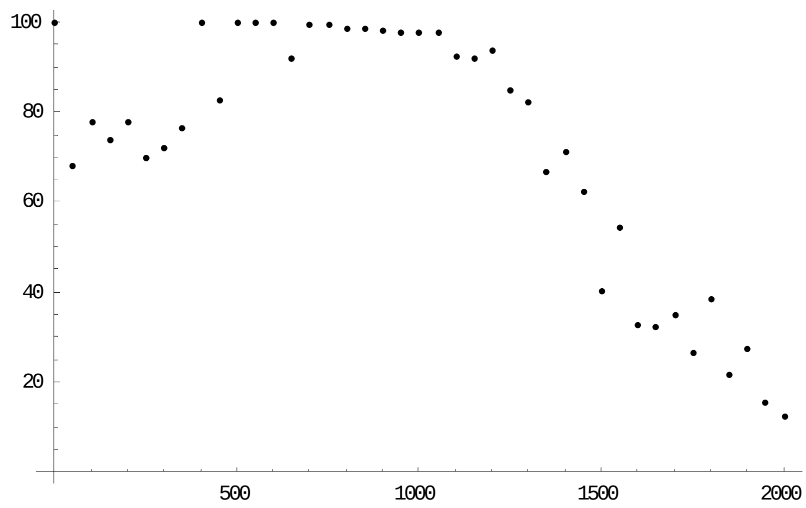
c) **In the magnetocaloric effect, the increase in magnetic entropy during an adiabatic demagnetization process is offset by a decrease in the lattice entropy, and the sample cools. Gadolinium gallium garnet, $Gd_3Ga_5O_{12}$, is used for very low temperature magnetic refrigeration (< 10 K) based on this effect. The change in magnetic entropy with the applied field is calculated through the Euler relation $\left(\frac{\partial M}{\partial T}\right)_H = \left(\frac{\partial S}{\partial H}\right)_T$. Make a plot of $\left(\frac{\partial M}{\partial T}\right)_H$ versus T for the values you found for the two fields. Based on your results, what operating temperature range will have the greatest change in magnetic entropy?**

From the graphs in part 1a and 1b, it is clear that the entropy will change most dramatically in the steep region just before the Curie temperature. Quantifying this by taking the absolute value of magnetization, averaging, then taking a numerical derivative one arrives at the plot:

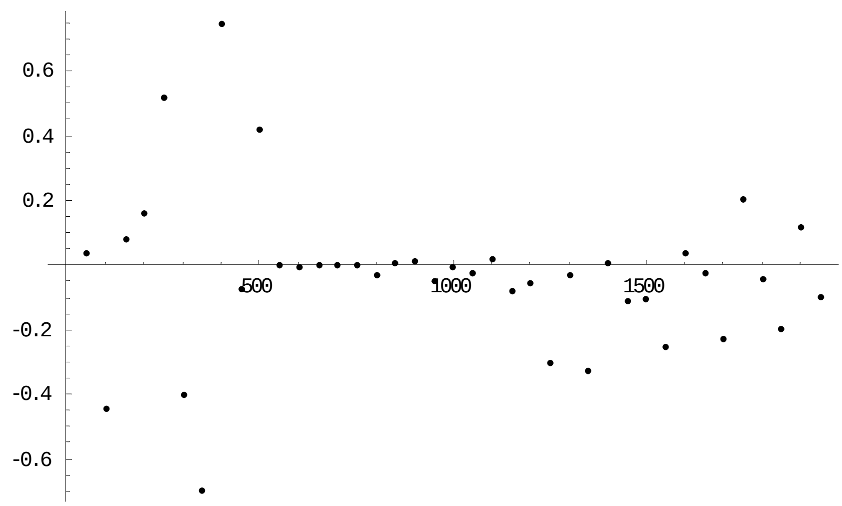
Plotting the absolute value of magnetization in units of "number of squares in the dominant orientation" versus temperature (Kelvin) or zero field, I have:



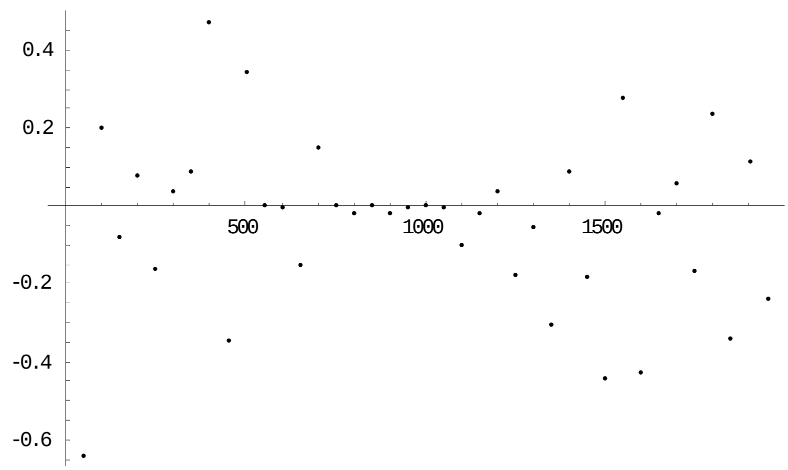
I see that it's pushed slightly higher in the case of a 0.01 Tesla field:



Please note that the drop near zero temperature is an artifact of not enough Monte Carlo steps, as discussed before. Note that in both of the graphs below, the derivative is in units of “change in total number of squares in the dominant orientation per Kelvin”. The derivative in the zero field case is then:



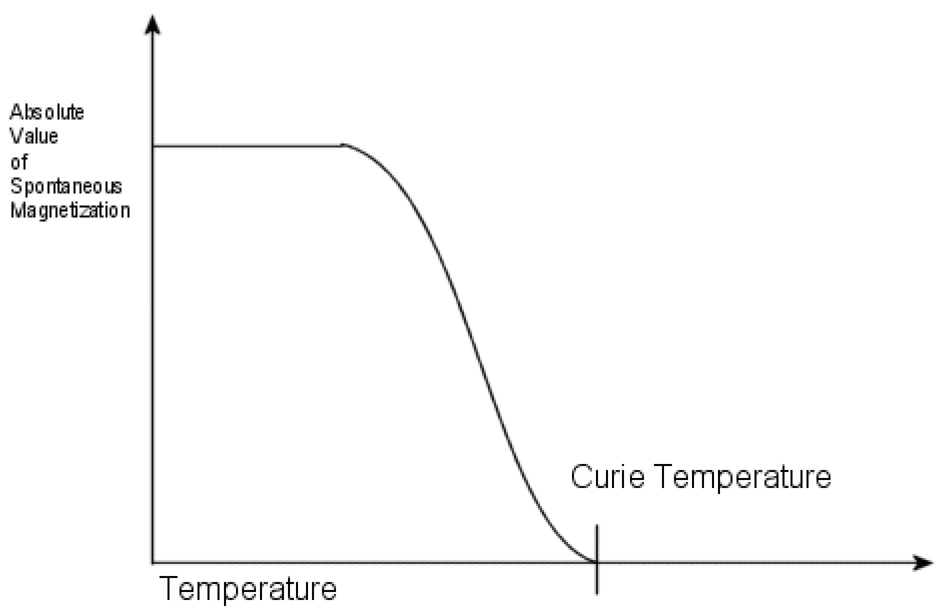
Namely, that the entropy is decreasing with field most heavily near the Curie temperature. In the case with a magnetic field applied, this decrease seems to be a bit steeper. Again, ignore the initial part of the plot, as this arises from insufficient equilibration time as described earlier.



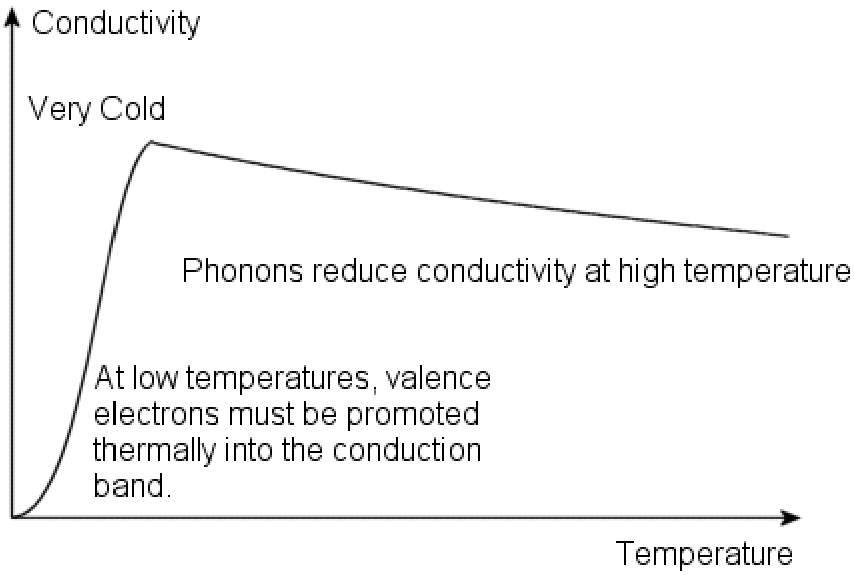
2) $La_xCa_{1-x}MnO_3$ **is a half-metallic (semimetal) ferromagnet. It is unusual because it has roughly the same critical temperature for an insulator-to-metal transition and for a ferromagnet-to-magnet transition. The combination of the two leads to what is called "Colossal" magnetoresistance.**

a) **Show using diagrams the temperature-dependent behavior of the spontaneous magnetization and electrical resistance.**

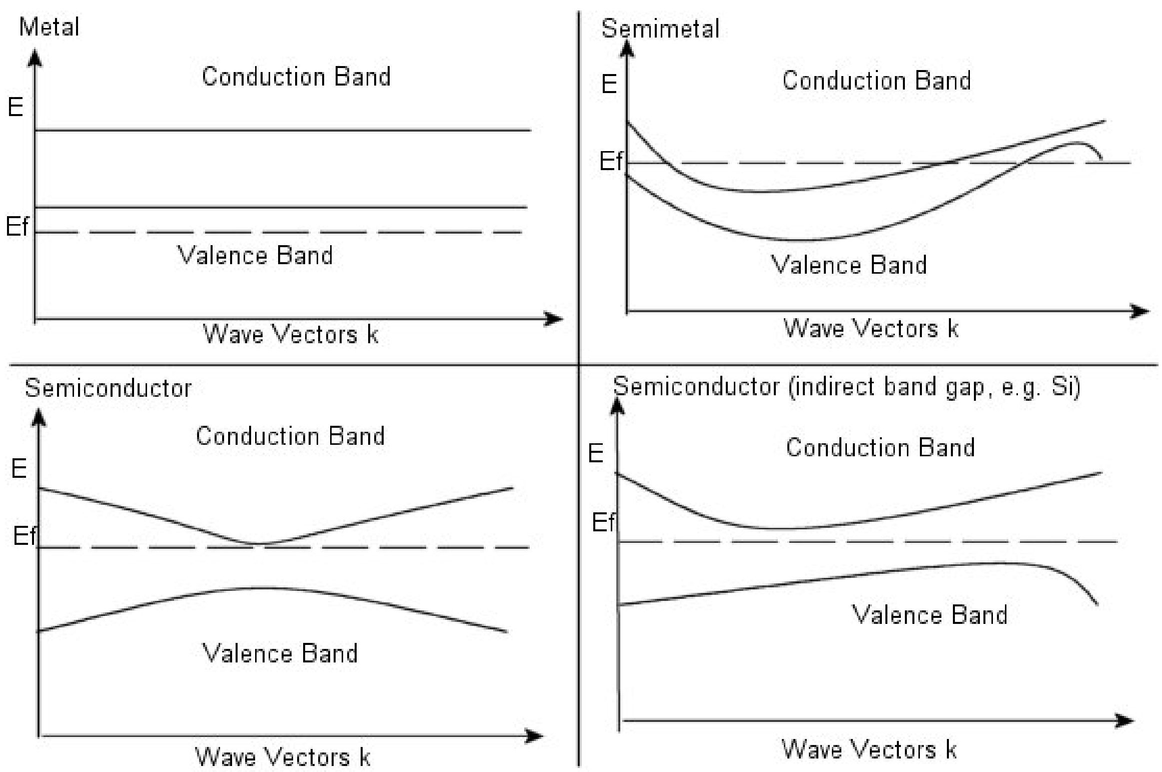
Spontaneous magnetization of a material decreases with temperature, as is shown experimentally in part 1:



At low temperatures, resistance decreases as electrons are thermally promoted into the conduction band (resistance later increases as phonons interfere with conduction).



b) Explain with simplified band structure diagrams how the electronic band structure gives rise to the properties described in part (a).



At very low temperatures, the electrons are all very strongly coupled in their valence orbitals. In terms of resistance, then, the material does not conduct until electrons reach the conduction band. Then, as the material becomes more thermally excited electrons begin to be promoted past the band gap and conductance rises.

In terms of ferromagnetism, this property arises from strong coupling between spins of unpaired valence electrons. At a sufficiently high temperature, then, valence electrons will be promoted both within the valence band and into the conduction band to such a degree so as to have very poor correlation between adjacent valence band electrons.

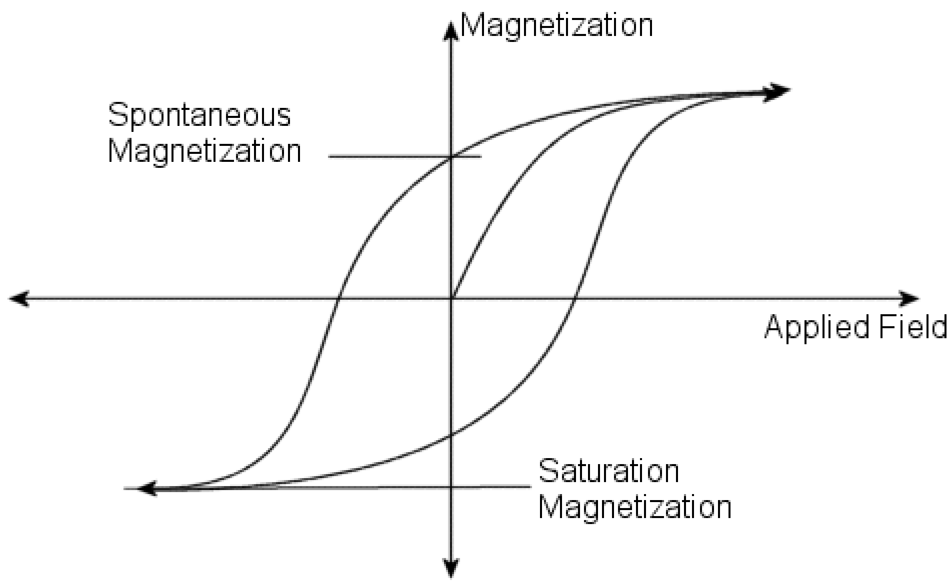
Note that if the conduction band is spin polarized in a semimetal, then it will be ferromagnetic as well as a small population of electrons may be promoted into the preferred spin band.

c) Suggest why a half-metallic ferromagnet might show a large change in the electrical resistivity at a fixed temperature when a magnetic field is applied.

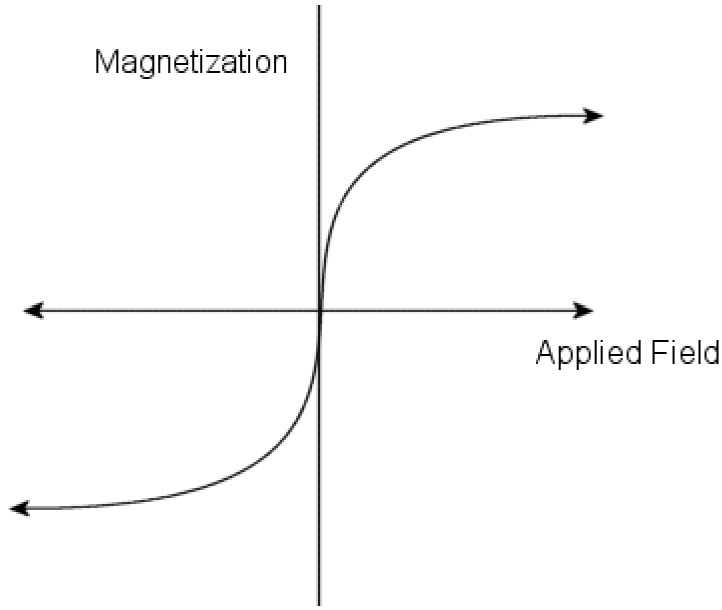
A plausible scenario would be as such: by applying a magnetic field, one causes a discrepancy between the energies of one spin versus another spin. By shifting the energies of spins, one could hypothetically draw electrons out of the conductance band and couple them into the valence band or alternatively push electrons up into the conductance band, depending on the position of the band gap, the Fermi energy, and the strength of the field.

This is facilitated, in this case, by the fact that at roughly the same temperature (energy $E = kT$), the band gap and the Curie temperature coincide so as to allow one of the two shifted spin energies to be suppressed in the band gap region.

d) Show what the M versus H curves look like for different temperature regions.



Above is a typical M versus H curve in the ferromagnetic case (this dominates at temperatures below the Curie temperature). As temperature rises, the strength of the interaction between nearby electron spins decreases and as such the graph shrinks with temperature: that is, the saturation magnetization tips of the graph move closer and closer to the origin.



Above is now the typical M versus H curve in the paramagnetic case, which dominates at higher temperatures. Magnetization is much weaker with respect to the applied field here, and no spontaneous magnetization exists. There is, however, still a saturation magnetization beyond which point more field is ineffective at increasing magnetization.

3) **Please give short (1-2 paragraphs, with diagrams) answers to the following:**

a) **In the paper we discussed about photomagnetic switching** (Ultrafast non-thermal control of magnetization by instantaneous photomagnetic pulses)**, explain what was measured and why the signal oscillated as a function of time. What is the underlying physics responsible?**

The samples of material in the paper about ultra-fast magnetic switching were kept at extremely low temperature and being very thin had a weak magnetic field of their own, causing measurement of their magnetization state to be very difficult. Further, timing at the femtosecond scale was governed by varying the distance between the laser source and the sample. In fact, then, whether a flip occurred had to be measured by checking the Faraday rotation, e.g., the orientation of the polarization of transmitted light, using the magneto-optical Faraday effect. The Faraday rotation shifted the orientation with respect to the expected orientation depending on the magnetic polarization of the material: if a spin-flip occurred, the excitation and subsequent relaxation of the iron atoms caused a sudden spike in Faraday rotation compared to a photon which would induce a magnetization in the current direction of the ferromagnetic field.

Further, the oscillations arose simply from precession of the atomic magnetizations over time, since a canted antiferromagnetic orientation was used in this case.

The underlying physics responsible was simply Faraday's Law working in reverse: whereas a changing magnetic field creates a rotating electric field, a rotating electric field can create a changing magnetic field (the "inverse Faraday effect"). By shining circularly-polarized laser light at a material, then, a magnetic field could be created in a material with a sufficiently high Verdet constant (relating the tendency for a circularly-polarized photon to rotate in the material).

b) Suppose you compare two samples of a ferromagnetic material. One is fully dense, and the other has a number of inclusions (internal pores). Describe how the saturation magnetization, the remnant magnetization, and the coercive field vary between the two samples, and why.

Saturation magnetism is property intrinsic to the magnetic atoms, so saturation magnetism per magnetic volume (as per the standard definition) is not affected by inclusions.

The remnant magnetism will be affected since, as seen in problem (1), the exchange couplings will be modified for atoms adjacent to a pore or impurity. However, it is unclear whether remnant magnetism will increase or decrease: it could increase due to reduction in exchange couplings, or increase due to pinning of the domain walls!

The coercive field, or the field necessary to bring the overall magnetism of a material on the upper or lower tracks of the hysteresis loop to zero, will be similarly affected since again the coupling strengths of adjacent spins would be reduced by the absence of some of the atoms, but pinning of domain walls could well increase the coercive field.