Magnetic properties of spin 1/2 system Masatsugu Sei Suzuki Department of Physics, SUNY at Binghamton (Date: September 06, 2018).

Here we discuss the magnetization, entropy and heat capacity of the spin 1/2 system in the presence of an external magnetic field.

1. Ground state and excited state in the presence of magnetic field

The spin magnetic moment of spin 1/2 is

$$\boldsymbol{\mu}_{s} = -\frac{2\mu_{B}}{\hbar} \boldsymbol{S} = -\mu_{B} \boldsymbol{\sigma}.$$

where

$$S = \frac{\hbar}{2}\sigma.$$

The Zeeman energy is given by

$$\hat{H} = -\hat{\boldsymbol{\mu}}_{s} \cdot \boldsymbol{B} = -(-\mu_{B}\hat{\boldsymbol{\sigma}}) \cdot \boldsymbol{B} = \mu_{B}\sigma_{z}B,$$

in the presence of an external magnetic field B.

(i) For
$$E = -\mu_B B$$
 (ground state)

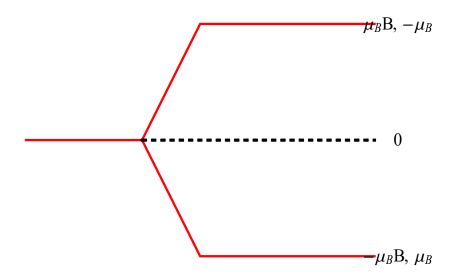
$$\sigma_z = -1, \qquad \mu_s = \mu_B$$

The direction of the magnetic moment is opposite to the direction of B

(ii) For
$$E = \mu_B B$$
 (excited state)

$$\sigma_z = 1$$
, $\mu_s = -\mu_B$

The direction of the magnetic moment is parallel to the direction of B



The energy gap is defined by

$$k_{\rm R}\Delta = 2\mu_{\rm R}B$$

where Δ is in the units of K.

The partition function

$$Z_N = Z^N$$

where N is the number of spins and Z is the partition function and is given by

$$Z = \exp(\frac{\mu_B B}{k_B T}) + \exp(-\frac{\mu_B B}{k_B T}) = 2\cosh(\beta \mu_B B)$$

2. Helmholtz energy

The Helmholtz free energy is

$$F = E - ST = -k_B T \ln Z_N = -k_B T N \ln Z$$

where E is the internal energy of the system and S is the entropy.

$$dF = dE - d(ST) = TdS - PdV - SdT - TdS = -PdV - SdT$$

In the magnetic system,

Intensive variable: $P \rightarrow M$

Extensive variable: $V \to H \text{ (or } V \to B)$

Then we get

$$dF = -MdB - SdT$$

or

$$M = -\frac{\partial F}{\partial B}, \qquad S = -\frac{\partial F}{\partial T}$$

3. Magnetization M

The total magnetization of N spins (spin 1/2) is

$$M = -\frac{\partial F}{\partial B} = N\mu_B \tanh(\frac{\mu_B B}{k_B T}).$$

This expression of M can be also derived as

$$M = N \frac{\mu_{B} \exp(\frac{\mu_{B}B}{k_{B}T}) + (-\mu_{B}) \exp(-\frac{\mu_{B}B}{k_{B}T})}{\exp(\frac{\mu_{B}B}{k_{B}T}) + \exp(-\frac{\mu_{B}B}{k_{B}T})} = N\mu_{B} \tanh(\frac{\mu_{B}B}{k_{B}T})$$

In the limit of $\frac{\mu_B B}{k_B T} \rightarrow 0$,

$$M \approx N \mu_B \frac{\mu_B B}{k_B T} = \frac{N \mu_B^2}{k_B} \frac{B}{T} = \frac{C}{T} B,$$

showing the Curie law, where C is the Curie constant.

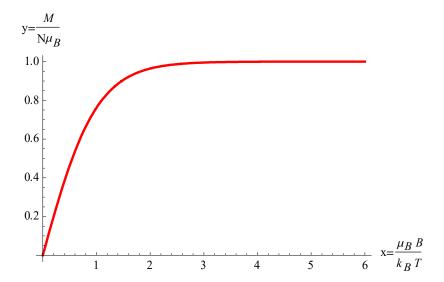


Fig. Scaling plot of the magnetization. The saturation magnetization is $N\mu_B$; y = 1.

4. Entropy S

The entropy is

$$\frac{S}{k_B N} = \ln[2\cosh(\frac{\mu_B B}{k_B T}) - \frac{\mu_B B}{k_B T} \tanh(\frac{\mu_B B}{k_B T}).$$

We introduce the characteristic temperature T_0 and magnetic field B_0 as

$$\mu_B B_0 = k_B T_0$$

Then we have

$$\frac{S}{k_B N} = \ln[2\cosh(\frac{\mu_B B}{k_B T}) - \frac{\mu_B B}{k_B T} \tanh(\frac{\mu_B B}{k_B T})$$
$$= \ln[2\cosh(\frac{b}{t}) - \frac{b}{t} \tanh(\frac{b}{t})$$

where

$$b = \frac{B}{B_0}, \qquad t = \frac{T}{T_0}$$

$$\frac{\mu_{B}B}{k_{B}T} = \frac{\mu_{B}B_{0}\frac{B}{B_{0}}}{k_{B}T_{0}\frac{T}{T_{0}}} = \frac{b}{t}$$

We make a plot of $\frac{S}{k_B N}$ as function of t, where b is changed as a parameter. In the limit of $t \to \infty$, the entropy reached

$$\frac{S}{k_B N} = \ln(2s+1) = \ln 2 = 0.693147.$$

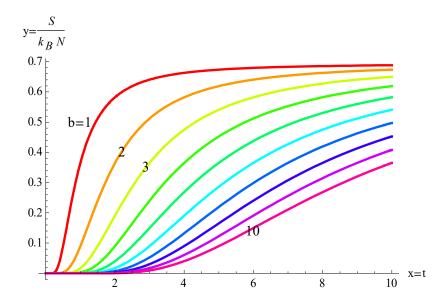


Fig. Plot of $\frac{S}{k_B N}$ as a function of a reduced temperature $t = T/T_0$, where the reduced magnetic field $b = B/B_0$ is changed as a parameter. Note that $\mu_B B_0 = k_B T_0$. The highest value of y is $\ln 2 = 0.693147$

5. Isentropic demagnetizion

The principle of magnetically cooling a sample is as follows. The paramagnet is first cooled to a low starting temperature. The magnetic cooling then proceeds via two steps.

Suppose that the spin system is kept at temperature T_1 in the presence of magnetic field B_1 . The system is insulated ($\Delta S = 0$) and the field removed, the system follows the constant entropy path AB, ending up at the temperature T_2 (isentropic process). If B_{Δ} is the effective field that corresponds to the local interactions, the final temperature T_2 reached in an isentropic demagnetization process is

$$\frac{T_2}{B_{\Lambda}} = \frac{T_1}{B_1} .$$

since the entropy is a function of only B/T.

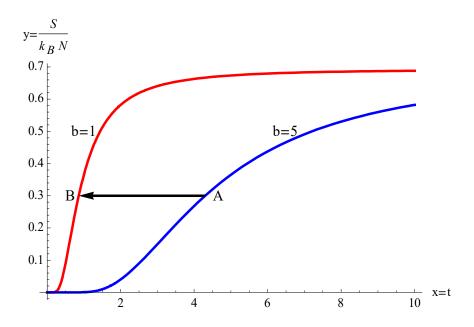


Fig. Point A ($t_A = 4.29726$, $y_A = 0.3$) on the line with $\frac{B_A}{B_0} = 1$. Point B ($t_B = 0.859452$, , $y_A = 0.3$) on the line with $\frac{B_B}{B_0} = 5$. The path AB is the isentropic process (y = 0.3). Note that

$$\frac{t_A}{B_A} = \frac{t_B}{B_B} .$$

6. Specific heat

The heat capacity is given by

$$\frac{C}{Nk_B} = \left(\frac{\mu_B B}{k_B T}\right)^2 \sec h^2 \left(\frac{\mu_B B}{k_B T}\right)$$

Using the energy gap parameter

$$k_B \Delta = 2 \mu_B B$$

$$\frac{C}{Nk_{R}} = (\frac{\Delta}{2T})^{2} \sec h^{2} (\frac{\Delta}{2T}) = \frac{1}{4} (\frac{\Delta}{T})^{2} \sec h^{2} (\frac{\Delta}{2T}) = \frac{1}{4} (\frac{\Delta}{T})^{2} \frac{e^{T/\Delta}}{(1 + e^{T/\Delta})^{2}}$$

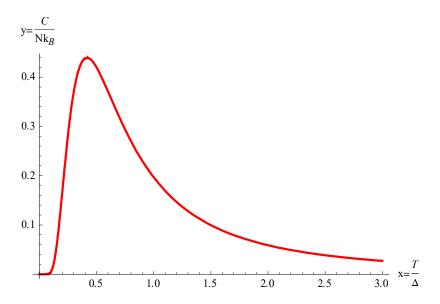


Fig. Plot of the heat capacity C/k_B as a function of T/Δ . It show a peak at $T/\Delta = 0.416778$.

The heat capacity as a function of temperature, has a peak at

$$\frac{T}{\Delta} = 0.416778.$$

((Schottky anomaly))

The Schottky anomaly is an observed effect in solid state physics where the specific heat capacity of a solid at low temperature has a peak. It is called anomalous because the heat capacity usually increases with temperature, or stays constant. It occurs in systems with a limited number of energy levels so that E(T) increases with sharp steps, one for each energy level that becomes available. Since Cv = (dE/dT), it will experience a large peak as the temperature crosses over from one step to the next.