Spin 1/2 system in magnetic field

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date: April 26, 2013).

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

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

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)

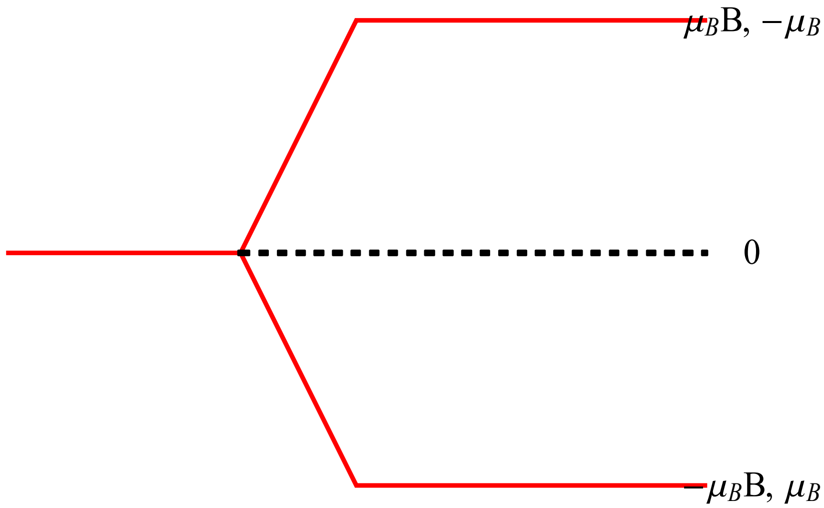
$$\sigma_z = -1, \qquad \mu_s = \mu_B$$

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

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

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: $P \to M$

Extensive variable: $V \to H$ (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 $\frac{\mu_B B}{k_B T} \to 0$,

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

showing the Curie law.

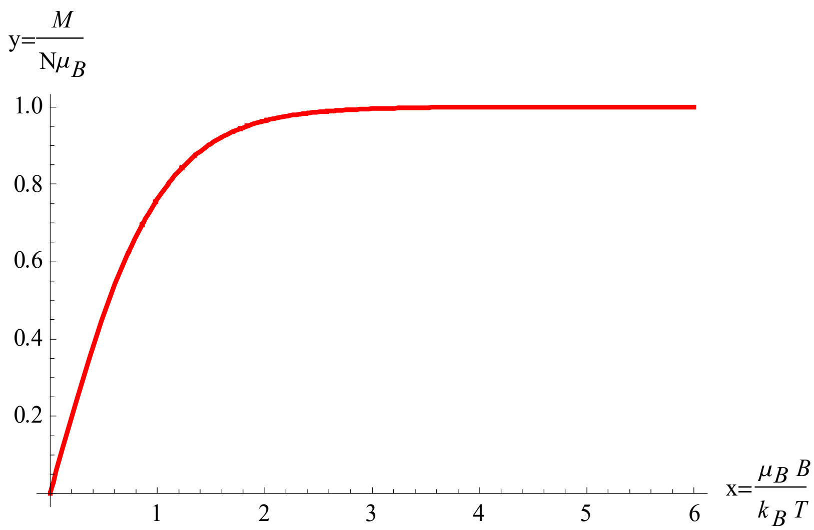


Fig. Scaling plot of the magnetization. The saturation magnetization is $N\mu_B$; $y = 1$.

4. Entropy *S*

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

We introduce the characteristic temperature T_0 and magnetic field B_0 as

$$\mu_B B_0 = k_B T_0$$

Then we have

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

where

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

$$\frac{\mu_B B}{k_B T} = \frac{\mu_B B_0 \dfrac{B}{B_0}}{k_B T_0 \dfrac{T}{T_0}} = \frac{b}{t}$$

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

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

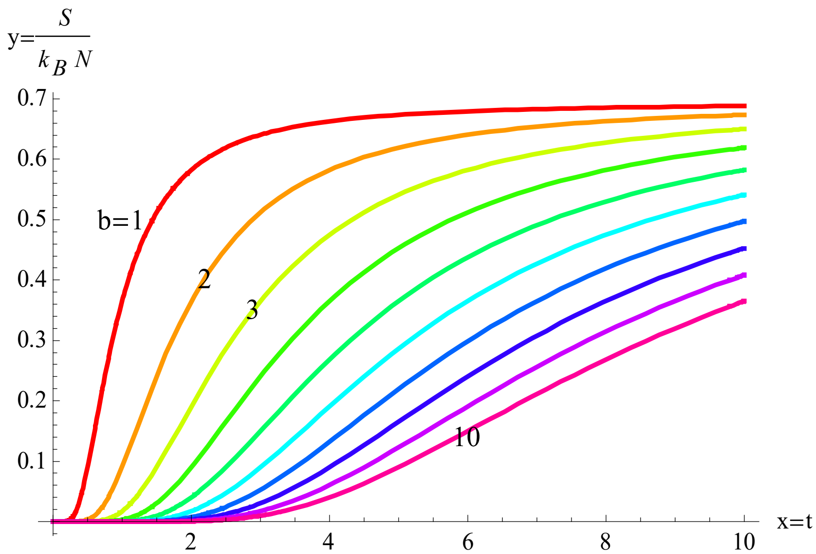


Fig. Plot of $\frac{S}{k_B N}$ as a function of a reduced temperature t (= T/T_0), where the reduced magnetic field b (= B/B_0) is changed as a parameter. Note that $\mu_B B_0 = k_B T_0$. The highest value of y is ln2 = 0.693147

5. Isentropic demagnetizion

The principle of magnetically cooling a sample is as follows. The paramagnet is first cooled toa 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

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

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

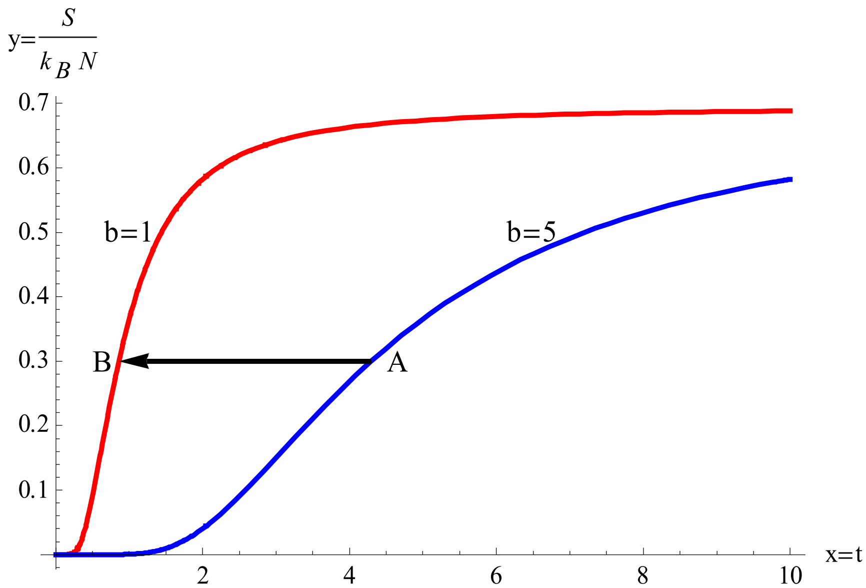


Fig. Point A (t_A = 4.29726, y_A = 0.3) on the line with $\frac{B_A}{B_0} = 1$. Point B (t_B= 0.859452, , y_A = 0.3) on the line with $\frac{B_B}{B_0} = 5$. The path AB is the isentropic process (y = 0.3). Note that

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

6. Specific heat

The heat capacity is given by

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

Using the energy gap parameter

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

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

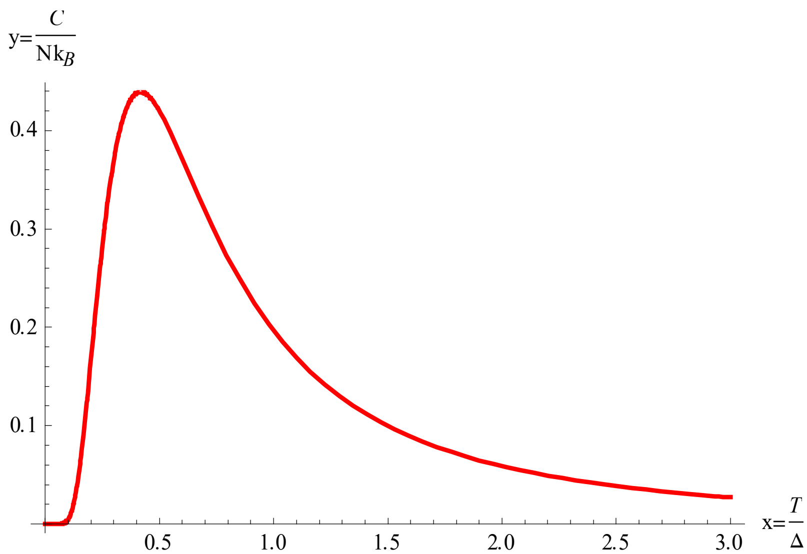


Fig. Plot of the heat capacity C/k_B as a function of T/Δ. It show a peak at $T/\Delta = 0.416778$.

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 $C_v = (dE/dT)$, it will experience a large peak as the temperature crosses over from one step to the next.