Magnetization with spin: the canonical ensemble

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1. Spin 1/2 states in the magnetic field

We consider the electron spin system with two energy levels in the presence of an external magnetic field B along the z axis. The spin magnetic moment $\boldsymbol{\mu}$ is given by

$$\boldsymbol{\mu} = -\frac{g\boldsymbol{S}}{\hbar}\mu_B = -\frac{2\boldsymbol{S}}{\hbar}\mu_B = -\mu_B\boldsymbol{\sigma} ,$$

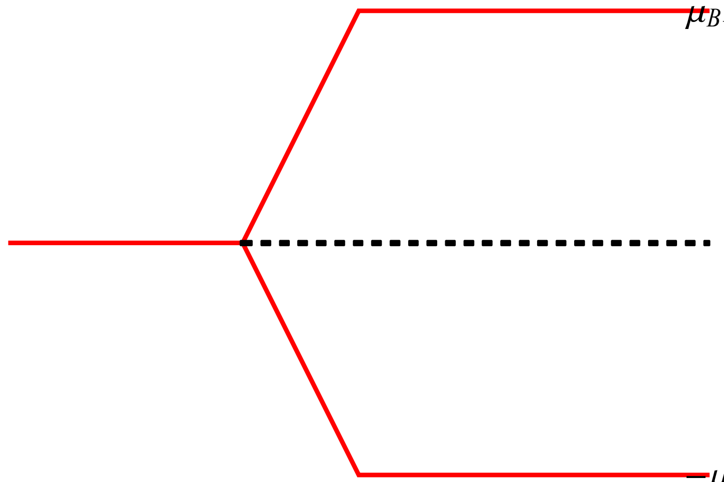
where g is the Landé g-factor (g = 2) for electron spin, $\boldsymbol{S}$ $(=\frac{\hbar}{2}\boldsymbol{\sigma})$ is the spin angular momentum, $\mu_B = \frac{e\hbar}{2mc}$ (>) is the Bohr magneton, and the charge of electron is –e (e>0). In the presence of the magnetic field along the z axis, we have a Zeeman energy given by

$$\varepsilon = -\boldsymbol{\mu}\cdot\boldsymbol{B} = -(-\mu_B\boldsymbol{\sigma})\cdot\boldsymbol{B} = \mu_B B\,\sigma_z$$

Noting that $\sigma_z\left|+z\right\rangle = \left|+z\right\rangle$ and $\sigma_z\left|-z\right\rangle = -\left|-z\right\rangle$ in quantum mechanics, the energy level splits into two levels, $\pm\mu_B B$.

(a) The energy $\mu_B B$ (higher level),
The spin state $\left|+z\right\rangle$. The spin magnetic moment is antiparallel to the z-axis $(-\mu_B)$. $\left|\downarrow\right\rangle$ state.

(b) The energy $-\mu_B B$ (lower level).
The spin state: $\left|-z\right\rangle$. The spin magnetic moment is parallel to the z-axis $(+\mu_B)$; $\left|\uparrow\right\rangle$ state.



In this system, the partition function for the canonical ensemble is given by

$$Z_{CN} = Z_{c1}(1)Z_{c1}(2)...Z_{c1}(N)$$

where Z_c(i) is the partition function for spin i and N is the number of spins. We assume that there is no interaction between spins. Since

$$Z_{c1}(1) = Z_{c1}(2) = ... = Z_{c1}(N)$$

we have

$$Z_{CN} = [Z_{c1}(1)]^N$$

$Z_{C1}(1)$ is the one-particle partition function and is given by

$$Z_{C1} = \exp(\beta\mu_B B) + \exp(-\beta\mu_B B) = 2\cosh(\beta\mu_B B).$$

The partition function for the N site system is

$$Z_{CN} = (1 + e^{\beta\varepsilon_0})^N$$

The magnetization M is given by

$$M = -k_B T \frac{\partial}{\partial B} \ln Z_{CN} = N\mu_B \tanh(\beta\mu_B B)$$

We note that the magnetization M can be also directly derived from the definition as

$$\frac{M}{N} = \mu_B P_+ - \mu_B P_-$$

P_+ and P_- are probabilities for finding the magnetic moment μ_B in the lower energy level and for finding the magnetic moment $-\mu_B$ in the upper level, respectively,

$$P_+ = \frac{e^{-(-\beta\mu_B B)}}{Z_{c1}} = \frac{e^{\beta\mu_B B}}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}},$$

$$P_- = \frac{e^{-\beta\mu_B B}}{Z_{c1}} = \frac{e^{-\beta\mu_B B}}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}}$$

Then we have the magnetization as

$$\begin{aligned} M &= N(\mu_B P_+ - \mu_B P_-) \\ &= N[\frac{\mu_B e^{\beta\mu_B B} + (-\mu_B)e^{-\beta\mu_B B}}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}}] \\ &= N\mu_B \tanh(\beta\mu_B B) \end{aligned}$$

which is the same as that derived using the Helmholtz free energy. For $\beta\mu_B B << 1$, using the Taylor expansion, we have

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

2. Angular momentum *J* state in the magnetic field

We consider a magnetic atom with angular momentum $\hbar\boldsymbol{J}$. Each atom has a magnetic moment $\boldsymbol{\mu} = -g\mu_B\boldsymbol{J}$, where g is the Landé g-factor. In the presence of a magnetic field along the z axis, the Zeeman energy is given by

$$\hat{H} = -\boldsymbol{\mu}\cdot\boldsymbol{B} = -(-g\mu_B\boldsymbol{J})\cdot\boldsymbol{B} = g\mu_B B\, J_z$$

Since

$$\hat{H}\left|j, m_j\right\rangle = \mu_B B\, m_j\left|j, m_j\right\rangle$$

$\left|j,m_j\right\rangle$ is the eigenket of the spin Hamiltonian $\left|j,m_j\right\rangle$ with the energy eigenvalue

$$g\mu_B B\, m_{\rm j}$$

where

$$m_j = -j, -j+1, \ldots., j \qquad (2j+1)$$

and the corresponding energy level and magnetic moment for the fixed m_j are

Energy level ($g\mu_B B\, m_{\rm j}$) and magnetic moment ($g\mu_B\, m_{\rm s}$)

$Z_{C1}(1)$ is the one-particle partition function and is given by

$$\begin{aligned} Z_{C1} &= \sum_{m_j=-j}^{j} e^{-\beta g \mu_B m_j B} \\ &= \sum_{m_j=-j}^{j} e^{-\frac{x}{j} m_j} \\ &= \operatorname{csch}\left(\frac{x}{2j}\right)\sinh\left(x+\frac{x}{2j}\right) \\ &= Z_{c1}(x) \end{aligned},$$

where

$$x = gj\beta\mu_B B$$

$P(m_s)$ is the probabilities for finding the magnetic moment $(-g\mu_B\, m_{\rm j})$ in the energy level ($g\mu_B B\, m_{\rm s}$)

$$P(m_j) = \frac{e^{-g\beta\mu_B m_j B}}{Z_{c1}},$$

Then we have the magnetization per magnetic atom as

$$\frac{M}{N} = \sum_{m_s=-j}^{j}(-g\mu_B\, m_j)P(m_j)$$

$$= g\mu_B \frac{\sum_{m_j=-j}^{j}(-m_j)e^{-g\beta\mu_B m_j B}}{\sum_{m_j=-j}^{j} e^{-g\beta\mu_B m_j B}}$$

$$= g\mu_B \frac{\sum_{m_j=-j}^{j}(-m_j)e^{-\frac{m_j}{j}x}}{\sum_{m_j=-j}^{j} e^{-\frac{m_j}{j}x}}$$

or

$$\frac{M}{N} = g\mu_B j\frac{d}{dx}\ln(\sum_{m_j=-j}^{j} e^{-\frac{m_j}{j}x}) = g\mu_B j\frac{d}{dx}\ln Z_{c1}(x)$$

leading to the final expression for the total magnetization

$$M = Ng\mu_B jB_j(x)$$

where $B_j(x)$ is called the Brillouin function

$$B_j(x) = \frac{2j+1}{2j}\coth(\frac{2j+1}{2j}x) - \frac{1}{2j}\coth(\frac{1}{2j}x)\,.$$

((**Note**)) **Mathematica**

```
Clear["Global`*"];

f1 = Sum[Exp[- mj/j x], {mj, -j, j}] //
   ExpToTrig // TrigFactor
```

$$\mathrm{Csch}\left[\frac{x}{2 j}\right] \mathrm{Sinh}\left[x + \frac{x}{2 j}\right]$$

```
h1 = D[Log[f1], x] // Simplify
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$$\frac{-\mathrm{Coth}\left[\frac{x}{2 j}\right] + (1 + 2 j)\, \mathrm{Coth}\left[x + \frac{x}{2 j}\right]}{2 j}$$

When $x = gj\beta\mu_B B << 1$, using the Taylor expansion, we have

$$B_j(x) = \frac{j+1}{3j}x - \frac{1}{45}\frac{(j+1)[(j+1)^2 + j^2]}{2j^3}x^3 + ...$$

The magnetic susceptibility is

$$M = Ng\mu_B j\frac{j+1}{3j}x = Ng\mu_B \frac{j+1}{3}gj\beta\mu_B B = \frac{Ng^2\mu_B{}^2}{3k_B T}j(j+1)$$