## Paramagnetism

(notes to be added at the end of the first paramagnetism lecture)

We obtained the mean magnetic moment of the specimen

$$M = N\mu \tanh\left(\frac{\mu B}{kT}\right)$$

We can obtain the same result from $Z$ quite easy. Start with

$$Z = \sum_{\substack{j_1=\pm\mu \\ \vdots \\ j_N=\pm\mu}}' e^{\beta(j_1+\dots+j_N)B}$$

and observe that

$$\left(\frac{\partial Z}{\partial B}\right)_{\beta,N} = \sum_{\text{all states}}' (j_1+\dots+j_N)\beta\, e^{\beta(j_1+\dots+j_N)B} =$$

at $\beta$ and $N$ fixed

$$= \sum_{\text{all states}}' (j_1+\dots+j_N)\beta\, \frac{e^{\beta(j_1+\dots+j_N)B}}{Z} \cdot Z = Z\beta M$$

$$\boxed{M = \frac{1}{\beta}\left(\frac{\partial \ln Z}{\partial B}\right)_{\beta,N}}$$

Because $Z$ is so important it has its own name: PARTITION FUNCTION ( $Z$ comes from the german ZUSTANDSSUMME = sum over states )

Also the mean energy of the specimen can be obtained from $Z$. In general, and not only for this paramagnetic problem, we have

$$\left(\frac{\partial Z}{\partial \beta}\right)_{*} = \frac{\partial}{\partial \beta}\left(\sum_j{}' e^{-\beta E_j}\right) =$$

$$= -\sum_j{}' E_j e^{-\beta E_j} = -Z\sum_j{}' E_j \frac{e^{-\beta E_j}}{Z} =$$

$$= -Z\langle E\rangle$$

$*$ all the other parameters are fixed

so

$$\boxed{\langle E\rangle = -\left(\frac{\partial \ln Z}{\partial \beta}\right)_{\text{FIXED PARAMETERS (except } \beta \text{ of course)}}}$$

For paramagnetism

$$\boxed{\langle E\rangle = -\left(\frac{\partial \ln Z}{\partial \beta}\right)_{B,N}}$$

Now it is simple to obtain $M$ and $\langle E\rangle$ because we computed $Z$

$$Z = 2^N \left[\cosh\left(\frac{\mu B}{kT}\right)\right]^N$$

To emphasize the parameters $T, N$ and $B$ we write

$$Z(T,N,B) = 2^N \left[\cosh\left(\frac{\mu B}{kT}\right)\right]^N$$

So

$$M = \frac{1}{\beta}\left(\frac{\partial \ln Z}{\partial B}\right)_{\beta,N} =$$

$$= \frac{1}{\beta}\frac{\partial}{\partial B}\left(N \ln 2 + N \ln\left[\cosh\left(\frac{\mu B}{kT}\right)\right]\right)\Bigg|_{\beta,N} =$$

$$= \frac{1}{\beta} N \frac{\frac{\mu}{kT}\sinh\left(\frac{\mu B}{kT}\right)}{\cosh\left(\frac{\mu B}{kT}\right)} \underset{\substack{\uparrow \\ \text{because} \\ \beta = \frac{1}{kT}}}{=} N\mu \tanh\left(\frac{\mu B}{kT}\right)$$

!

So we have a standard way of computing mean values: take de partial derivative of

$$\ln Z$$

with respect to a desired variable.

Find now the <u>mean energy</u>

$$\langle E \rangle = -\left(\frac{\partial \ln Z}{\partial \beta}\right)_{B,N} =$$

$$= -\frac{\partial}{\partial \beta}\left(N \ln 2 + N \ln\left[\cosh(\mu\beta B)\right]\right)\Big|_{B,N} =$$

$$= -N \frac{\mu B \sinh(\mu\beta B)}{\cosh(\mu\beta B)}$$

$$\boxed{\langle E \rangle = -N\mu B \tanh(\mu\beta B)}$$

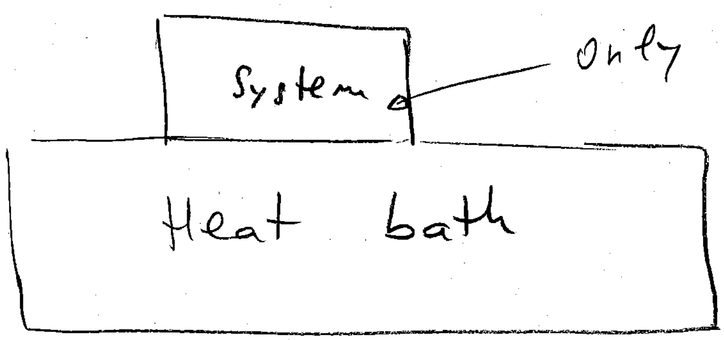
We can invert the relation

$$\langle E \rangle = -N\mu B \tanh(\mu \beta B)$$

to find $\beta$ in terms of $\langle E \rangle$

$$\beta = \frac{1}{\mu B} \operatorname{artanh}\left(-\frac{\langle E \rangle}{N\mu B}\right)$$

In other words, if you know the <u>average</u> energy you know $\beta$.




Only $\langle E \rangle$ is fixed by the temperature of the Heat bath.

<u>Back to the first postulate</u>

$$S = -k_B \sum_j p_j \ln p_j$$

given

$$\langle E \rangle = \sum_j p_j E_j \qquad (1)$$

$$1 = \sum_j p_j \qquad (2)$$

Find $p_1, \ldots, p_N$ so $S$ is maximum given the constraints (1) and (2)

To solve the problem we introduced two Lagrange multipliers $\alpha$ and $\beta$ (unknown at this point) and use the constraints by maximizing the combination (we simplifed the Boltzmann constant $k_B$ for algebraic convenience only)

$$\sum p_j \ln p_j - \alpha \sum p_j - \beta \sum p_j E_j$$

In the past lecture we got

$$\begin{cases} e^{1+\alpha} = \sum_j e^{-\beta E_j} & (1) \\ \langle E \rangle = \sum E_j \dfrac{e^{-\beta E_j}}{Z} & (2) \end{cases}$$

With $\langle E \rangle$ and $E_j$ given this is a system of two equations for the two unknowns $\alpha$ and $\beta$. Usually it is difficult to solve it. However for our paramagnetic case we can solve it. We found

$$\beta = \frac{1}{\mu B} \operatorname{artanh}\left(-\frac{\langle E \rangle}{N\mu B}\right) \quad (3)$$

from (2). The parameter $\alpha$ is given by (1)

$$e^{\alpha} = \frac{1}{e} \sum_j e^{-\beta E_j} = \frac{1}{e} Z = \frac{2^N}{e} \left[\cosh(\beta \mu B)\right]^N$$

and you can insert $\beta$ from (3) into