Paramagnetism (canonical ensemble)

→ macroscopic magnetic behavior from the collective behavior of microscopic magnetic moments

→ paramagnetism: materials in which there is no spontaneous magnetization, but magnetization can be made finite by placing a sample under a finite field ⇒ $M = M(B)$

in paramagnets M points in the same direction as B

- model: individual moments ⇒ their sum gives the total magnetization

$$H = -\sum_{i=1}^{N} \vec{\mu}_i \cdot \vec{B}$$

⇒ $\vec{B}$ - external field
$\vec{\mu}_i$ - individual moment

→ $\vec{\mu} = \gamma \vec{J}$ ($\vec{J}$ ≡ angular momentum)

$\vec{\mu}$ - magnetic moment originates from the spin and angular momentum of electrons on individual atoms simplest case: spin-1/2 system

$$\vec{S} = \frac{\vec{\sigma}}{2}$$

$$H = -\sum_i \gamma \vec{S}_i \cdot \vec{B} \qquad \gamma \text{- gyromagnetic ratio}$$

$$Z_N = \operatorname{Tr} e^{-\beta H}$$

1.) Z_N factorizes into single-spin terms

$$Z_N = \left[\operatorname{Tr} e^{-\beta h}\right]^N \qquad h = \gamma \vec{S} \cdot \vec{B}$$

2.) No $N!$ factor $\Rightarrow$ spins are on different sites $\Rightarrow$ distinguishable

$h = \gamma \vec{S} \cdot \vec{B} \rightarrow$ assume z-direction $\rightarrow h = \gamma S_z \cdot B_z$

$$h|+\rangle = \frac{\gamma}{2} B_z |+\rangle$$

$$h|-\rangle = -\frac{\gamma}{2} B_z |-\rangle$$

$$Z_N = \left[e^{-\beta\frac{\gamma B_z}{2}} + e^{\beta\frac{\gamma B_z}{2}}\right]^N$$

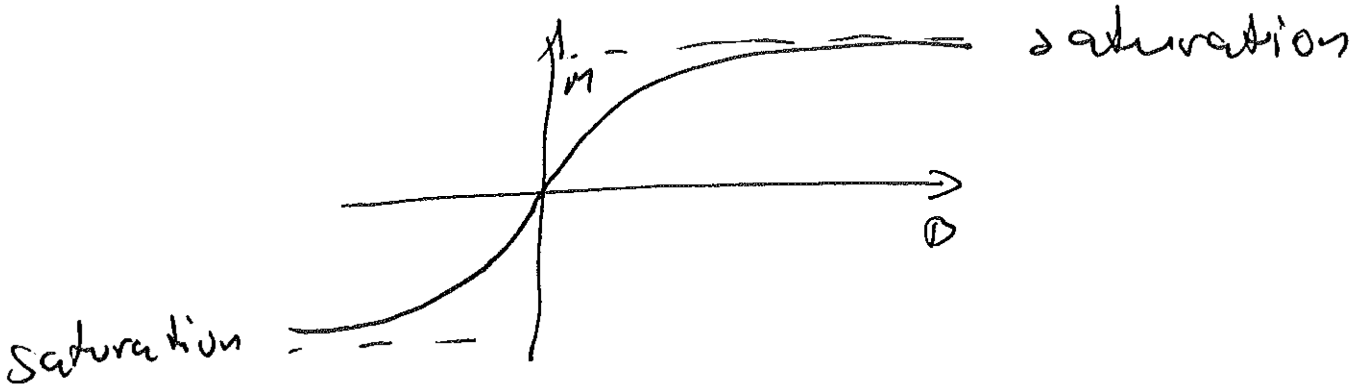
$$B = B_z$$

$$Z_N = 2^N \cosh \frac{\beta \gamma B}{2}$$

average energy: $\bar{E} = -\frac{\partial \ln Z}{\partial \beta} = -\frac{\sinh\left(\frac{\beta\gamma B}{2}\right)}{\cosh\left(\frac{\beta\gamma B}{2}\right)} \frac{\gamma B N}{2}$

average magnetization: $\bar{m} = \frac{1}{\beta}\frac{\partial \ln Z}{\partial B} = \tanh\left(\frac{\beta\gamma B}{2}\right)\frac{\gamma N}{2}$

or $\boxed{\bar{m} = N\mu \tanh\left(\frac{\beta \cancel{\gamma} B \mu}{2}\right)}$



- for a finite field as $B \to 0$ or $T \to \infty$

$$M = \frac{N\mu^2 B}{kT}$$

for large $T \Rightarrow F = E - TS \Rightarrow$ entropy plays an enhanced role $\Rightarrow$ destroys alignment with the magnetic field

- susceptibility:

$$\frac{\partial M}{\partial B} = \frac{N\mu^2}{kT}$$

- application: magnetic resonance imaging

Paramagnetism / Micro canonical ensemble

For comparison: let's work this out !!!

* spin-1/2 system in magnetic field $(0,0,B_z)$

$$H = -\sum_i \vec{\mu}_i \cdot \vec{B} = -\sum_i \vec{\mu}_z^{(i)} \cdot B_z$$

spins are either up or down

$$\cancel{\vec{\mu}_z^{(i)} B_z |+\rangle = \mu B |+\rangle}$$

$\vec{\mu}_z^{(i)}$

- can count the number of states with a given energy:

  - N-sites

    $N_\uparrow$ - number of sites with up-spin

$$E[N_\uparrow, N] = N_\uparrow \mu B - (N - N_\uparrow)\mu B$$
$$= 2N_\uparrow \mu B - N\mu B \Rightarrow \frac{E + N\mu B}{2\mu B} = N_\uparrow$$

$$\Omega(E) = \frac{N!}{N_\uparrow!\,(N-N_\uparrow)!}$$

entropy: $S = k \ln \Omega(E)$

using Stirling approximation

$$\frac{S}{k} = N\ln N - N_\uparrow \ln N_\uparrow - (N - N_\uparrow)\ln(N - N_\uparrow)$$
$$\frac{S}{k} = N\ln N - \left(\frac{E + N\mu B}{2\mu B}\right)\ln\left(\frac{E + N\mu B}{2\mu B}\right) - \left(\frac{N\mu B - E}{2\mu B}\right)\ln\left(\frac{N\mu B - E}{2\mu B}\right)$$

calculate temperature

$$\frac{1}{T} = \frac{\partial S}{\partial E} = -\frac{k}{2\mu B}\ln\left(\frac{E + N\mu B}{2\mu B}\right) + \frac{k}{2\mu B}\ln\left(\frac{N\mu B - E}{2\mu B}\right)$$

$$1 = \frac{kT}{2\mu B}\ln\left(\frac{N\mu B - E}{N\mu B + E}\right)$$

$$\Rightarrow \quad e^{\frac{2\mu B}{kT}} = \frac{N\mu B - E}{N\mu B + E}$$

$$e^{\frac{2\mu B}{kT}} (N\mu B + E) = N\mu B - E$$

$$\boxed{E = N\mu B \frac{\left(1 - e^{\frac{2\mu B}{kT}}\right)}{\left(1 + e^{\frac{2\mu B}{kT}}\right)} = \underline{N\mu B \tanh\left(\frac{\mu B}{kT}\right)}}$$

same as canonical!!!

magnetisation

$\cancel{\bar{M} = T \frac{\partial S}{\partial B}}$?

$$\bar{M} = T \frac{\partial S}{\partial B}$$

rewrite entropy as:

$$\frac{S}{k} = N \ln N - \left(\frac{E}{2\mu B} + \frac{N}{2}\right) \ln\left(\frac{E}{2\mu B} + \frac{N}{2}\right)$$

$$- \left(\frac{N}{2} - \frac{E}{2\mu B}\right) \ln\left(\frac{N}{2} - \frac{E}{2\mu B}\right)$$

$$\frac{\partial S}{\partial B} = - \frac{Ek}{2\mu B^2} \ln\left(\frac{E}{2\mu B} + \frac{N}{2}\right)$$

$$\cancel{- (1) \left(-\frac{E}{2\mu B^2}\right)}$$

$$+ \frac{E}{2\mu B^2} \ln\left(\frac{N}{2} - \frac{E}{2\mu B}\right)$$

$$\cancel{- (1) \left(\frac{E}{2\mu B^2}\right)}$$

$$\frac{\partial S}{\partial B} = \frac{Ek}{2\mu B^2} \ln\left(\frac{N\mu B - E}{N\mu B + E}\right) = \frac{\cancel{2} E k}{\cancel{2}\mu B^2} \frac{\mu B}{kT}$$

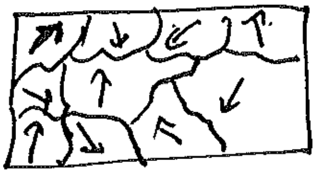
$$\boxed{\bar{M} = T \frac{\partial S}{\partial B} = \frac{N\mu}{\cancel{2}} \tanh\left(\frac{\mu B}{kT}\right)}$$

Ferromagnetism and the Ising model

paramagnetism: collective exogenous effect

- atomic magnetic moments are totally independent
- system described by $\hat{H} = -\sum_i \vec{\mu}_i \cdot \vec{B}$; cannot reproduce effects such as ferromagnetism, hysteresis
- ferromagnetic substances: below T_c system orders into ferromagnetic state (above $T_c \rightarrow$ paramagnetic)
  - ferromagnetic ordered state: magnetization which occurs spontaneously in the absence of a magnetic field
  - microscopically: magnetic moments are not independent $\Rightarrow$ they align with each other

    endogenous effect
- actually in a ferromagnetic ordered state it can happen that the measured magnetization is zero $\Rightarrow$ but in this case there would be finite macroscopic domains with finite magnetization in different directions



$\Rightarrow$ can average to zero

Ising model: $H = -\sum_{\langle i,j \rangle} J_{ij}\,\sigma_i \sigma_j - B \sum_i \sigma_i$

$J_{ij} \rightarrow$ interaction between spins (often nearest neighbor)

$\sigma_i \rightarrow$ spins $\Rightarrow$ can take value ± 1

partition function: $Z_N = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} e^{\beta H}$

- must sum over all configurations

$\sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1}$

i.e. $\Rightarrow$ over all different spin states of each lattice site

* lattices can be of various types: square, triangular, hexagonal, etc. ... (in 2D)

* Ising model can be solved easily in 1D
  can be solved not so easily in 2D
  until now can not be solved in 3D

* we will solve ~~for~~ it in 1D using
  - canonical ensemble
  - microcanonical ensemble

Ising model in 1D canonical ensemble

$$H = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1}$$

$$(B = 0)$$

J - nearest neighbor coupling

$$Z_N(T) = \sum_{\sigma_1} \dots \sum_{\sigma_N} e^{\beta J \sum_i \sigma_i \sigma_{i+1}}$$

periodic boundary conditions (ring)

$$H = -J \left[\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \dots + \underline{\sigma_N \sigma_1} \right]$$

$$Z_N(T) = \bar{\bar{T}}^N$$

$\bar{\bar{T}}$ - transfer matrix

$\sigma_{i+1} \backslash \sigma_i$	$+1$	-1
$+1$	$e^{\beta J}$	$e^{-\beta J}$
-1	$e^{-\beta J}$	$e^{\beta J}$

$$\hat{T} = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix}$$

$$Z_N(T) = \lambda_0^N + \lambda_1^N = \lambda_0^N \left(1 + \left(\frac{\lambda_1}{\lambda_0} \right)^N \right)$$

$\lambda_0, \lambda_1 \Rightarrow$ two eigenvalues of $\bar{\bar{T}}$

$$\lambda_1 < \lambda_0$$

diagonalize $\bar{\bar{T}}$

$$\begin{vmatrix} e^{\beta J}-\lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J}-\lambda \end{vmatrix} = 0$$ 1D

$$\Rightarrow \quad (e^{\beta J}-\lambda)^2 = e^{-2\beta J}$$

$$e^{\beta J}-\lambda = \pm e^{-\beta J}$$

$$\lambda = 2\cosh\beta J,\ 2\sinh\beta J$$

$$2\cosh\beta J \geq 2\sinh\beta J$$

$$Z_N(T) = 2^N \cosh^N \beta J$$

average energy: $\bar{E} = -\dfrac{\partial \ln Z_N}{\partial \beta} = -\dfrac{1}{Z_N}\dfrac{\partial Z_N}{\partial \beta}$

$$\frac{\partial Z_N}{\partial \beta} = 2^N N(\cosh^{N-1}\beta J)(\sinh(\beta J))J$$

$$\bar{E} = -NJ\tanh(\beta J)$$

specific heat $C = \dfrac{\partial \bar{E}}{\partial \beta}\dfrac{\partial \beta}{\partial T} = -NJ\left(1 - \tanh^2(\beta J)\right)J\left(\dfrac{\partial \beta}{\partial T}\right)$

$$= \frac{NJ^2\left(1-\tanh^2(\beta J)\right)}{kT^2} \Rightarrow \text{continuous function!}$$

no phase transition!

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if B-field is finite same procedure can be applied $\Rightarrow$ done in the book $\Rightarrow$ shown that there is no phase transition

Ising model, 1D, Microcanonical Ensemble

$$H = -J \sum_i \sigma_i \sigma_{i+1}$$

bonds can be ~~either~~ connecting either parallel or antiparallel spins →

total energy: $E = -J N_p + J N_a$

N_p → number of bonds with parallel spins ↑↑ or ↓↓

N_a → number of bonds with anti-parallel spins ↑↓ or ↓↑

we know that $N = N_p + N_a$

N - number of sites or number of bonds

$$E = -J N_p + J(N - N_p) = JN - 2J N_p$$

$$N_p = \frac{JN - E}{2J}$$

number of configurations: $\Omega(N_p) = \dfrac{N!}{N_p!\,(N-N_p)!}$

$$\Omega(N_p) = N\ln N - N_p\ln N_p - (N-N_p)\ln(N-N_p)$$

$$N_p = \frac{JN-E}{2J}$$

$$N - N_p = \frac{JN+E}{2J}$$

$$S = k \cancel{\ln}\left[N\ln N - \left(\frac{JN-E}{2J}\right)\ln\left(\frac{JN-E}{2J}\right) - \left(\frac{JN+E}{2J}\right)\ln\left(\frac{JN+E}{2J}\right)\right]$$

$$\frac{1}{T} = \frac{\partial S}{\partial E} \Rightarrow \frac{\partial S}{\partial E} = \left[\frac{1}{2J}\ln\left(\frac{JN-E}{2J}\right) - \frac{1}{2J}\ln\left(\frac{JN+E}{2J}\right)\right]k$$

$$\frac{2J}{kT} = \ln\left(\frac{JN-E}{JN+E}\right)$$

$$(JN+E)\, e^{2J/kT} = JN - E$$

$$E(e^{2J/kT}+1) = JN(1-e^{2J/kT})$$

$$E = -JN\tanh(2J/kT)$$