HH0032 Ferromagnetism

I would start with a no-go theorem, showing magnetism is a quantum effect and cannot be described by classical physics.

① Bohr-van Leeuwen theorem:

Consider a system of N electrons, the magnetic moment of each electron is $\boxed{\vec{m} = \frac{1}{2} q \vec{r} \times \vec{v}}$

$\vec{m}$ is a "linear" function of velocity $\vec{v}$! It means the total magnetic moment $\vec{M}$ is also a linear function of all velocities $\vec{v}_i$. For instance, the z component can be written in the following form,

$$\boxed{M_z = \sum_{i=1}^{3N} a_i(q_1, q_2, \cdots, q_{3N})\, \dot{q}_i}$$

generalized velocity

a_i doesn't depend on p_i ☺

The Hamiltonian is $\quad H = \sum_{i=1}^{N} \frac{1}{2m} (\vec{p}_i - q\vec{A})^2 + qV(q_1 \cdots q_{3N})$

And, the EOM's are $\quad \boxed{\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad -\dot{p}_i = \frac{\partial H}{\partial q_i}}$

Thus, we can rewrite the magnetic moment as,

$$M_z = \sum_{i=1}^{3N} a_i(q_1 \cdots q_{3N}) \frac{\partial H}{\partial p_i}$$

From Boltzmann distribution, the magnetic moment can be computed,

$$\boxed{\langle M_z \rangle = \frac{\int dq_i \int dp_i \, M_z e^{-H/\tau}}{\int dq_i \int dp_i \, e^{-H/\tau}}}$$

focus on the numerator ⊙⊙"

numerator $= \int dq_1 \cdots dq_{3N} \sum_{i=1}^{3N} a_i(q_1 \cdots q_{3N}) \int dp_1 \cdots dp_{3N} \frac{\partial H}{\partial p_i} e^{-H/\tau}$

note that $\int_{-\infty}^{+\infty} dp_i \frac{\partial H}{\partial p_i} e^{-H/\tau} = -\tau e^{-H/\tau} \Big|_{p_i=-\infty}^{+\infty} = 0$!!

As a result, the numerator vanishes! It means the total magnetic moment is identically zero

$$\langle M_z \rangle = 0 \,!$$ ← Bohr-van Leeuwen theorem.

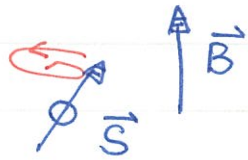
② Spin, the quantum spin ...

$\vec{m} = \frac{q}{2}\vec{r}\times\vec{v}$ $\qquad$ $\vec{m} = g\mu_B\vec{S}$

It turns out that there is another way to generate magnetic moment — spin!

$$\boxed{\vec{m} = g\mu_B\vec{S}}$$

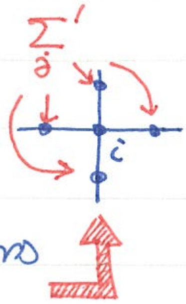
— It is not surprising that a spin interacts with an external magnetic field $U = -\vec{m}\cdot\vec{B} = -g\mu_B\vec{S}\cdot\vec{B}$

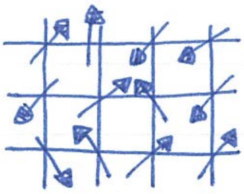


— Different spins also interact with each other through the exchange coupling $U_{int} = -J\,\vec{S}_1\cdot\vec{S}_2$

Combine both interactions together → We know how to write down the Hamiltonian for a ferromagnet.

$$\boxed{H = -\frac{J}{2}\sum_i \sum_j{}' \vec{S}_i\cdot\vec{S}_j - g\mu_B\sum_i \vec{S}_i\cdot\vec{B}}$$





spins in 2D

Note that $\sum_j{}'$ sums over all neighbors of site i and the factor of $\frac{1}{2}$ is to avoid double counting.

For simplicity, let me focus on $s=\frac{1}{2}$ spins.

$$\boxed{\vec{S} = (S_x, S_y, S_z) = \left(\frac{\hbar}{2}\sigma_x, \frac{\hbar}{2}\sigma_y, \frac{\hbar}{2}\sigma_z\right)}$$

$\sigma_x, \sigma_y, \sigma_z$ are Pauli matrices.

To your mental comfort, these matrices are explicitly written out,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Let us simplify the spin Hamiltonian a bit.

$$\boxed{H = \frac{-\varepsilon}{2} \sum_i {\sum_j}' \vec{\sigma}_i \cdot \vec{\sigma}_j - h \sum_i \sigma_i^z}$$

Here we choose $\vec{B} = (0,0,B)$

$\varepsilon = \frac{1}{4}\hbar^2 J$ dimensionless $h = \frac{1}{2}\hbar g \mu_B B$

Both ε and h have the unit of energy. Furthermore, introduce raising/lowering operators, $\sigma^{\pm} \equiv \frac{1}{2}(\sigma_x \pm i\sigma_y)$

$$\sigma_i^x \sigma_j^x = (\sigma_i^+ + \sigma_i^-)(\sigma_j^+ + \sigma_j^-) = \sigma_i^+\sigma_j^- + \sigma_i^-\sigma_j^+ + \sigma_i^+\sigma_j^+ + \sigma_i^-\sigma_j^-$$

$$\sigma_i^y \sigma_j^y = -(\sigma_i^+ - \sigma_i^-)(\sigma_j^+ - \sigma_j^-) = \sigma_i^+\sigma_j^- + \sigma_i^-\sigma_j^+ - \sigma_i^+\sigma_j^+ - \sigma_i^-\sigma_j^-$$

$$\longrightarrow \boxed{\sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y = 2(\sigma_i^+\sigma_j^- + \sigma_i^-\sigma_j^+)}$$

useful identity.

Now we can separate the Hamiltonian into two parts:

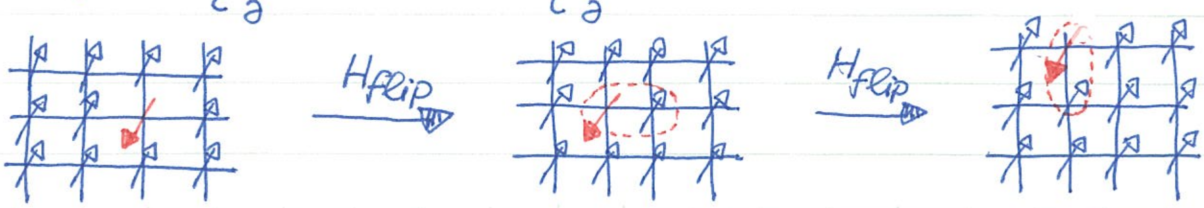
$$H_{Ising} = \frac{-\varepsilon}{2} \sum_i {\sum_j}' \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^z$$

contains only σ^z terms

$$H_{flip} = -\varepsilon \sum_i {\sum_j}' (\sigma_i^+\sigma_j^- + \sigma_i^-\sigma_j^+)$$

$\sigma^{\pm}$ terms.

$$\begin{cases} \sigma_i^+\sigma_j^- \,|\cdots \underset{i}{\downarrow} \underset{j}{\uparrow} \cdots\rangle = |\cdots \underset{i}{\uparrow} \underset{j}{\downarrow} \cdots\rangle & \text{flip } (\downarrow\uparrow) \text{ to } (\uparrow\downarrow) \\ \sigma_i^-\sigma_j^+ \,|\cdots \underset{i}{\uparrow} \underset{j}{\downarrow} \cdots\rangle = |\cdots \underset{i}{\downarrow} \underset{j}{\uparrow} \cdots\rangle & \text{flip } (\uparrow\downarrow) \text{ to } (\downarrow\uparrow) \end{cases}$$



H_{flip} acts like the kinetic energy of a down spin in the sea of up spins. (see previous figure). Because it is not easy to handle, we just drop it here.

⑦ Ferromagnetic phase transition.

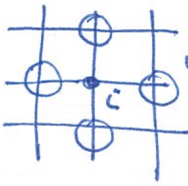
The σ_z-term Hamiltonian is the so-called Ising model,

$$\underline{H_{Ising} = \frac{-\varepsilon}{2} \sum_i \sum_j{}' \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^z}$$

Because all σ_i^z commute, it is equivalent to ignore the matrix structure and just treat all σ_i^z as c-numbers.

$$\boxed{E_{Ising} = \frac{-\varepsilon}{2} \sum_i \sum_j{}' \sigma_i \sigma_j - h \sum_i \sigma_i} \qquad \sigma_i = \pm 1$$

Focus on a particular spin σ_i. It's energy is



j sites

$z=4$, number of neighbors

$$E_i = -\varepsilon \sum_j{}' \sigma_j \sigma_i - h\sigma_i$$

mean-field approximation.

$$\approx \underline{-\varepsilon z \langle\sigma\rangle \sigma_i - h\sigma_i}$$

Within the mean-field approximation, it seems that the spin σ_i feels an effective magnetic field,

simple ☺

$$\boxed{h_{eff} = \underbrace{\varepsilon z \langle \sigma \rangle}_{\text{molecular field}} + \underbrace{h}_{\text{external field}}} \quad \text{and} \quad \boxed{E_i = -h_{eff}\sigma_i}$$

We can proceed to compute the average $\langle\sigma\rangle$ self-consistently.

$$\langle \sigma_i \rangle = \frac{(+1)e^{h_{eff}/\tau} + (-1)e^{-h_{eff}/\tau}}{e^{h_{eff}/\tau} + e^{-h_{eff}/\tau}} = \underline{\tanh(h_{eff}/\tau)}$$

But, we expect $\langle\sigma_i\rangle = \langle\sigma\rangle$ is uniform in a ferromagnet.

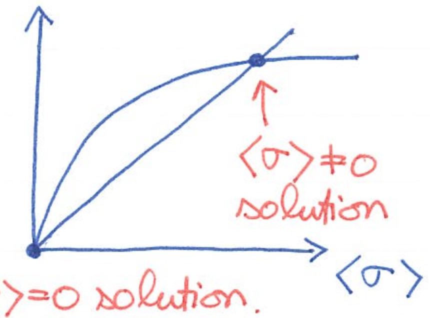
In the absence of magnetic field ($h=0$), the self-consistent equation is

$$\boxed{\langle\sigma\rangle = \tanh\left[\frac{\varepsilon z}{\tau}\langle\sigma\rangle\right]}$$

finally

Introduce the critical temperature $\tau_c = \varepsilon z$. For $\tau < \tau_c$, the value of $\langle\sigma\rangle$ can be obtained by finding intersection of the curves on both sides:

$\tau < \tau_c$



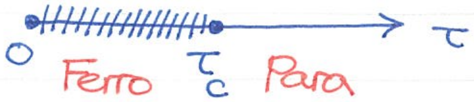
The self-consistent equation gives two solutions. It turns out that only $\langle\sigma\rangle \neq 0$ solution is stable for $\tau < \tau_c$ $\longrightarrow$ ferromagnet!!

On the other hand, the situation changes when $\tau > \tau_c$.

$\tau > \tau_c$

Only $\langle\sigma\rangle = 0$ solution exists. The spin system does not exhibit any spontaneous magnetic moment in the absence of magnetic field.

Phase diagram:



The mean-field theory shows that the spin system goes through a ferro-para phase transition when τ is changed.

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