



UNIVERSITY OF STRASBOURG

Exam — Session 1

T. Charitat, J. Farago, G. Weick

Transcribed by
PIERRE GUICHARD

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1 Ferromagnetism and antiferromagnetism

Let us consider a d -dimensional Ising model, consisting of $N \gg 1$ Ising spins $s_i = \pm 1$ at the temperature T , located at the sites i of a hypercubic lattice and subject to a magnetic field h (in energy units). We denote $\beta = 1/k_B T$, with k_B the Boltzmann constant. In what follows, we only consider interactions between nearest neighbors. The Hamiltonian of the system is written as

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_{i=1}^N s_i, \quad (1.1)$$

where $\langle i, j \rangle$ denotes a summation over nearest neighbors i and j .

1.1 Ferromagnetism and mean-field approximation

In this first part of the problem, the coupling constant J is positive and we denote it $J = J_F$, with $J_F > 0$.

(a) Justify that within the mean field approximation,

$$s_i s_j \simeq (s_i + s_j)m - m^2 \text{ for } i \neq j,$$

where $m = \langle s_i \rangle$ is the average magnetization per site.

We can always decompose a variable as the sum of its mean value and the fluctuations around the mean value,

$$s_i = \langle s_i \rangle + \delta s_i = m_i + \delta s_i$$

$$\begin{cases} s_i = m + \delta s_i \\ s_j = m + \delta s_j \end{cases}$$

$$\begin{aligned} s_i s_j &= m^2 + m(\delta s_i + \delta s_j) + \underbrace{\delta s_i \delta s_j}_{\approx 0} \\ &= m^2 + m(s_i - m + s_j - m) \\ &= m(s_i + s_j) - m^2 \end{aligned}$$

(b) Deduce that within the above-mentioned approximation, the Hamiltonian (1.1) takes the form

$$H \simeq -(h + zJ_F m) \sum_{i=1}^N s_i + \frac{1}{2} N z J_F m^2, \quad (1.2)$$

with z the number of nearest neighbors of a given lattice site i .

We can now rewrite,

$$\begin{aligned}
 H &= -J_F \sum_{\langle i,j \rangle} s_i s_j - h \sum_{i=1}^N s_i \\
 &\approx -J_F \sum_{\langle i,j \rangle} [(s_i + s_j)m - m^2] - h \sum_{i=1}^N s_i \\
 &= -J_F m \underbrace{\sum_{\langle i,j \rangle} (s_i + s_j)}_{\text{dummy index}} + J_F m^2 \underbrace{\sum_{\langle i,j \rangle} 1}_{=\frac{1}{2}Nz} - h \sum_{i=1}^N s_i \\
 &= -2J_F m \underbrace{\sum_{\langle i,j \rangle} s_i}_{=\frac{1}{2}z \sum_{i=1}^N s_i} + \frac{1}{2}Nz J_F m^2 - h \sum_{i=1}^N s_i \\
 &= -(h + zJ_F m) \sum_{i=1}^N s_i + \frac{1}{2}Nz J_F m^2
 \end{aligned}$$

Which is exactly the (1.2) hamiltonian.

- (c) What is the physical meaning of the term $h + zJ_F m$ in the mean-field Hamiltonian (1.2)?

The term $h + zJ_F m$ has the meaning of an *effective field* by spin i . It takes into account the interactions between i and its first neighbors, and account the field disturbance that this implies.

- (d) Calculate the canonical partition function Z and the free energy F of the system within the mean-field approximation.

We know that the partition function Z is,

$$\begin{aligned}
Z &= \sum_{s_1} \cdots \sum_{s_N} e^{-\beta H} \\
&= \sum_{s_1} \cdots \sum_{s_N} e^{\beta \left[(h+zJ_F m) \sum_{i=1}^N s_i - \frac{1}{2} N z J_F m^2 \right]} \\
&= e^{-\frac{\beta}{2} N z J_F m^2} \sum_{\{s_k\}} \prod_{i=1}^N e^{\beta (h+zJ_F m) s_i} \\
&= e^{-\frac{\beta}{2} N z J_F m^2} \prod_{i=1}^N \sum_{\{s_i=\pm 1\}} e^{\beta (h+zJ_F m) s_i} \\
&= e^{-\frac{\beta}{2} N z J_F m^2} \prod_{i=1}^N [2 \cosh(\beta (h+zJ_F m))] \\
&= e^{-\frac{\beta}{2} N z J_F m^2} [2 \cosh(\beta (h+zJ_F m))]^N
\end{aligned}$$

And the free energy F ,

$$\begin{aligned}
F &= -k_B T \ln Z \\
&= -k_B T \ln \left\{ e^{-\frac{\beta}{2} N z J_F m^2} [2 \cosh(\beta (h+zJ_F m))]^N \right\} \\
&= \frac{N z J_F m^2}{2} - N k_B T \ln [2 \cosh(\beta (h+zJ_F m))]
\end{aligned}$$

- (e) Show that the average magnetization m per site is the solution of a self-consistent equation that you will explicitly determine. (Do not discuss the general possible solutions.)

We know that,

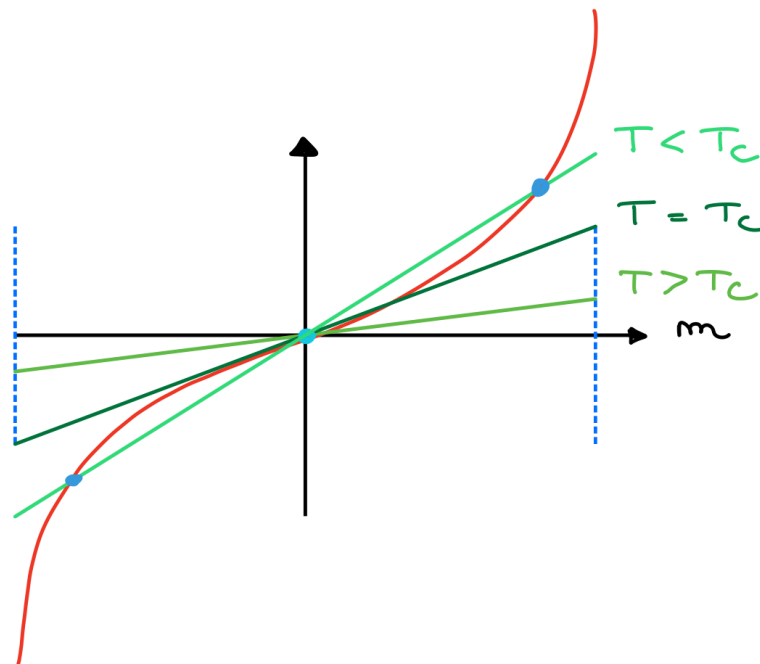
$$m = -\frac{\partial F}{\partial h} = \tanh(\beta (h+zJ_F m))$$

- (f) Let us consider for this question that $h = 0$. Show that there exists a phase transition (paramagnetic-ferromagnetic) for a critical temperature T_c . Determine T_c as a function of the different parameters of the problem. What does the mean-field approximation predict for the case $d = 1$? Compare to your knowledge of the exact solution of the one-dimensional Ising model.

For $h = 0$,

$$m = \tanh(\beta z J_F m)$$

We can solve this equation graphically,



we can write,

$$\operatorname{arctanh}(m) = \beta z J_F m$$

We define a critical temperature T_c defined by,

$$k_B T_c = z J_F$$

The mean-field approximation predict a phase transition in $d = 1$, however, we know that this is wrong when we're doing the exact calculation for the $d = 1$ Ising model (without any approximations). This is due of the fact that, Ising model start being good as the number of nearest neighbors start to be huge, in the 1D case, there is not enough neighbors to perform such an approximation and expect to have correct results.

1.2 Antiferromagnetism

In this second part of the problem, the coupling constant is negative, and we denote it $J = -J_{AF}$ with $J_{AF} > 0$.

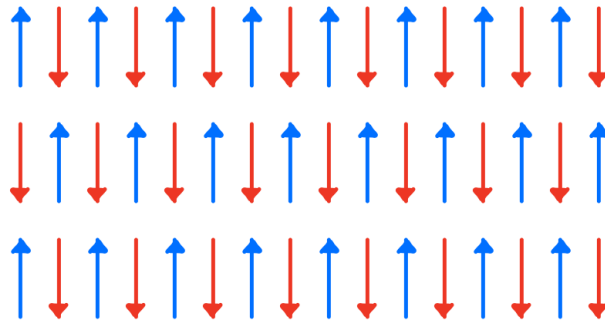
1.2.1 General results

- (a) Describe the effect of the first term of the Hamiltonian 1.1 on the spin orientations.

Now the hamiltonian is,

$$\mathcal{H} = J_{AF} \sum_{\langle i,j \rangle} s_i s_j - h \sum_{i=1}^N s_i$$

Now this first term, instead of enforcing spin's alignment, will force spin's anti-alignment, as shown on this schematic



- (b) Let us consider for this question that $T = 0$ and $h = 0$. Justify that the system splits into two sublattices A and B , such that the spins take the value $+1$ or -1 depending on the sublattice to which they belong. These states are called *Néel states*. How many Néel states are there? Give the expressions of the magnetization and the average energy of the Néel states.

As shown on the schematic, the first term of the hamiltonian will force the anti-alignment of the spins, so, at null-temperature, the whole lattice will be anti aligned. We can then consider two sub-lattices, one representing spin up \uparrow and the other one the spin down \downarrow . There is as much Néel states as there is of distinct spin state. In our case there is only two states : $+1$ and -1 , therefore two Néel states.

- (c) Still at $T = 0$, what is the qualitative effect of a positive uniform magnetic field h ? By comparing the energy of a Néel state subject to a finite magnetic field and that of a ferromagnetic state (where all the spins are orientated in the same direction), deduce the critical value h_c ($T = 0$) for which it is possible for the system to go from the antiferromagnetic phase to the ferromagnetic one.

1.2.2 Mean-field approximation

We call $m_A = \langle s_i \rangle$ ($i \in A$) the average magnetization of the spins belonging to the sublattice A and $m_B = \langle s_j \rangle$ ($j \in B$) the average magnetization of the spins belonging to the sublattice B .

- (a) Justify that

$$s_i s_j \simeq s_i m_B + s_j m_A - m_A m_B \quad (i \in A, j \in B)$$

in the mean-field approximation.

As we did before,

$$\begin{cases} s_i = \langle s_i \rangle + \delta s_i = m_A + \delta s_i \\ s_j = \langle s_j \rangle + \delta s_j = m_B + \delta s_j \end{cases}$$

$$\begin{aligned}
s_i s_j &= (m_A + \delta s_i)(m_B + \delta s_j) \\
&= m_A m_B + m_A \delta s_j + m_B \delta s_i + \underbrace{\delta s_i \delta s_j}_{\approx 0} \\
&= m_A m_B + m_A + m_A (s_j - m_B) + m_B (s_i - m_A) \\
&= s_i m_B + s_j m_A - m_A m_B
\end{aligned}$$

(b) Deduce from the preceding question that one can approximate the Hamiltonian (1.1) by

$$\begin{aligned}
H &\simeq -(h - zJ_{AF}m_B) \sum_{i \in A} s_i - (h - zJ_{AF}m_A) \sum_{j \in B} s_j - \frac{1}{2}NzJ_{AF}m_A m_B. \\
H &= -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_{i=1}^N s_i \\
&\approx J_{AF} \sum_{\langle i,j \rangle} (s_i m_B + s_j m_A - m_A m_B) - h \sum_{i=1}^N s_i \\
&= J_{AF} m_B \underbrace{\sum_{\langle i,j \rangle} s_i}_{=\frac{1}{2}z \sum_{i \in A} s_i} + J_{AF} m_A \underbrace{\sum_{\langle i,j \rangle} s_j}_{=\frac{1}{2}z \sum_{j \in B} s_j} - J_{AF} m_A m_B \underbrace{\sum_{\langle i,j \rangle} 1}_{=\frac{1}{2}Nz} - h \sum_{i=1}^N s_i \\
&= \frac{1}{2} J_{AF} m_B z \sum_{i \in A} s_i + \frac{1}{2} J_{AF} m_A z \sum_{j \in B} s_j - \frac{1}{2} N z J_{AF} m_A m_B - h \underbrace{\sum_{i=1}^N s_i}_{\sum_{i \in A} s_i + \sum_{j \in B} s_j} \\
&= -(h - zJ_{AF}m_B) \sum_{i \in A} s_i - (h - zJ_{AF}m_A) \sum_{j \in B} s_j - \frac{1}{2} N z J_{AF} m_A m_B
\end{aligned}$$

(c) Using your answers to questions 1.1(c) and 1.1(e), argue that m_A and m_B verify the following system of self-consistent equations :

$$\begin{aligned}
m_A &= \tanh(\beta[h - \lambda m_B]), \\
m_B &= \tanh(\beta[h - \lambda m_A]).
\end{aligned}$$

What is the expression of the constant λ ?

From 1.1(c) we know that, $h + zJ_F m$ was an effective field by spin i , now, we have in a way, two effective field, $h - zJ_{AF}m_B$ that act on spin i and $h - zJ_{AF}m_A$ that act on spin j . And from 1.1(e), the self consistent equation for m was,

$$m = \tanh(\beta(h + zJ_F m))$$

So in our situation,

$$\begin{cases} m_A = \tanh(\beta(h - zJ_{AF}m_B)) \\ m_B = \tanh(\beta(h - zJ_{AF}m_A)) \end{cases}$$

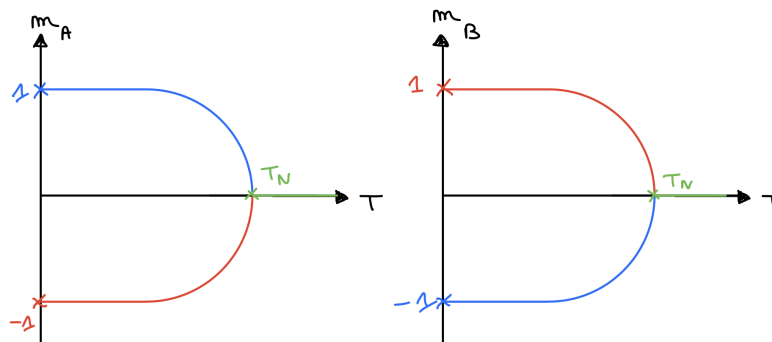
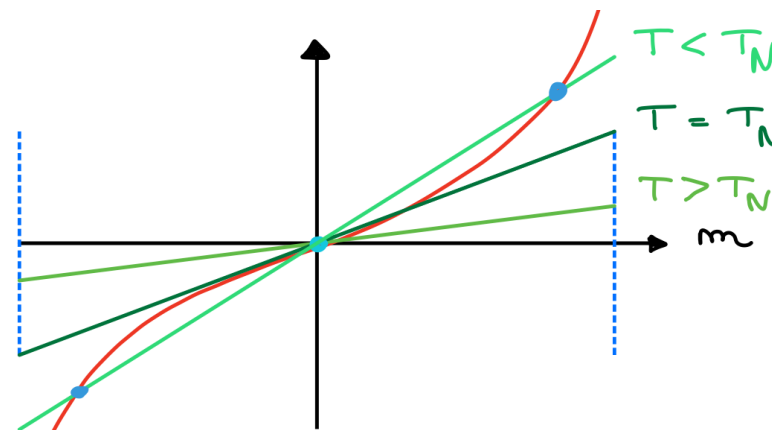
(d) Let us first consider the zero magnetic field case ($h = 0$).

- (i) Assuming that $m_A = -m_B$, show that there exists a phase transition for a temperature T_N (called the Néel temperature) between a phase where $m_A = -m_B = 0$ and a phase where $m_A(T) = -m_B(T) = m_0(T)$. Give an expression for T_N . Sketch $m_A(T)$ as a function of temperature.

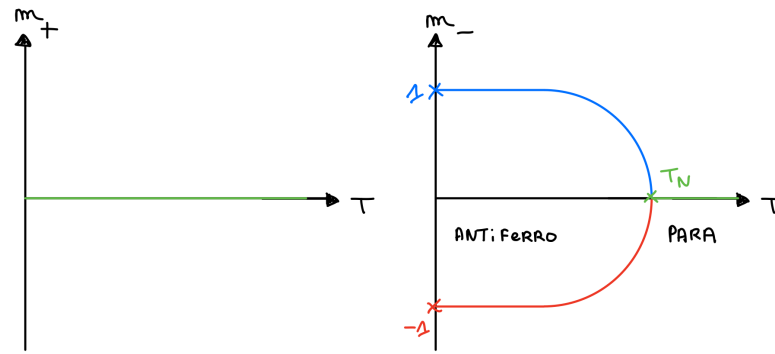
$$\begin{cases} m_A = \tanh(\beta(h - zJ_{AF}m_B)) \\ m_B = \tanh(\beta(h - zJ_{AF}m_A)) \end{cases} \implies \begin{cases} m_A = \tanh(\beta zJ_{AF}m_A) \\ m_B = \tanh(\beta zJ_{AF}m_B) \end{cases}$$

Which is the same equation for m_A and m_B , so we can use the result of the question 1.1(f), we can define the Néel temperature as,

$$k_B T_N = zJ_{AF}$$



- (ii) Sketch $m_+ = (m_A + m_B)/2$ and $m_- = (m_A - m_B)/2$ as a function of T . Which quantity is the order parameter of the antiferromagnetic-paramagnetic phase transition? What would you find if you would measure the average magnetization of the sample?



The quantity that is the order parameter of the antiferromagnetic-paramagnetic phase transition is m_- . The average magnetization of the sample at a given temperature T is $\langle m_-(T) \rangle$.

- (e) We now seek to characterize the effect of the magnetic field on m_A and m_B by calculating the magnetic susceptibility of the crystal defined by

$$\chi = \left. \frac{\partial m_+}{\partial h} \right|_{h=0}$$

- (i) We first consider that $T > T_N$ and we assume that the magnetic field is weak (with respect to what?). Linearize the self-consistent equations and show that

$$\chi(T) = \frac{C}{k_B T + k_B T_N} \quad (1.3)$$

where C is a dimensionless constant that you will determine.

$$\begin{cases} m_A = \tanh(\beta[h - zJ_{AF}m_B]) \approx \frac{h}{k_B T} - \frac{T_N}{T} m_B, \\ m_B = \tanh(\beta[h - zJ_{AF}m_A]) \approx \frac{h}{k_B T} - \frac{T_N}{T} m_A. \end{cases}$$

So,

$$m_+ = \frac{1}{2}(m_A + m_B) = \frac{h}{k_B T} - \frac{T_N}{2T}(m_A + m_B) = \frac{h}{k_B T} - \frac{T_N}{T} m_+$$

So,

$$m_+ \left(1 + \frac{T_N}{T} \right) = \frac{h}{k_B T}$$

So,

$$m_+ = \frac{h/k_B}{T + T_N}$$

So,

$$\begin{aligned}\chi &= N \left. \frac{\partial m_+}{\partial h} \right|_{h=0} \\ &= \frac{N/k_B}{T + T_N}\end{aligned}$$

So,

$$C = \frac{N}{2k_B}$$

- (ii) We now move to the case $T < T_N$. We assume that the magnetic field *his* weak and we write the magnetizations on the sites A and B as $m_A = m_0 + \Delta m_A$ and $m_B = -m_0 + \Delta m_B$, with $\Delta m_A \ll m_0$ and $\Delta m_B \ll m_0$. By performing a Taylor expansion of the self-consistent equations, show that the susceptibility takes the form ¹

$$\chi(T) = \frac{1}{k_B T \cosh^2\left(\frac{T_N}{T} m_0(T)\right) + k_B T_N} \quad (1.4)$$

Show that for $T > T_N$ one finds the previous result of Eq. (1.3). How does χ behave at low temperature? Sketch the graph of $\chi(T)$ and compare it to that of a ferromagnet.

$$m_A = \tanh\left(\frac{h}{k_B T} - \frac{T_N}{T} m_B\right) = \tanh\left(\frac{h}{k_B T} - \frac{T_N}{T} \Delta m_B + \frac{T_N}{T} m_0\right)$$

So,

$$m_0 + \Delta m_A \simeq \tanh\left(\frac{T_N}{T} m_0\right) + \frac{\frac{h}{k_B T} - \frac{T_N}{T} \Delta m_B}{\cosh^2\left(\frac{T_N}{T} m_0\right)}$$

And,

$$m_B = \tanh\left(\frac{h}{k_B T} - \frac{T_N}{T} m_A\right) = \tanh\left(\frac{h}{k_B T} - \frac{T_N}{T} \Delta m_A - \frac{T_N}{T} m_0\right)$$

So,

$$-m_0 + \Delta m_B \simeq -\tanh\left(\frac{T_N}{T} m_0\right) + \frac{\frac{h}{k_B T} - \frac{T_N}{T} \Delta m_A}{\cosh^2\left(\frac{T_N}{T} m_0\right)}$$

So,

$$m_A + m_B = \frac{\frac{2h}{k_B T} - \left(\frac{T_N}{T} \Delta m_A + \Delta m_B\right)}{\cosh^2\left(\frac{T_N}{T} m_0\right)} = \Delta m_A + \Delta m_B$$

1. We recall that $\tanh(a+x) \simeq \tanh a + x/\cosh^2 a$ for $x \ll 1$.

$$(\Delta m_A + \Delta m_B) \left\{ 1 + \frac{T_N}{T} \frac{1}{\cosh^2 \left(\frac{T_N}{T} m_0 \right)} \right\} = \frac{\frac{2h}{k_B T}}{\cosh^2 \left(\frac{T_N}{T} m_0 \right)}$$

Therefore,

$$\Delta m_A + \Delta m_B \equiv 2m_+ = \frac{2h}{k_B T \cosh^2 \left(\frac{T_N}{T} m_0 \right)} \cdot \frac{1}{1 + \frac{T_N}{T} \frac{1}{\cosh^2 \left(\frac{T_N}{T} m_0 \right)}} = \frac{2h}{k_B} \left\{ \frac{1}{T_N + T \cosh^2 \left(\frac{T_N}{T} m_0 \right)} \right\}$$

Meaning,

$$m_+ = \frac{h}{k_B} \left\{ \frac{1}{T_N + T \cosh^2 \left(\frac{T_N}{T} m_0 \right)} \right\}$$

So,

$$\chi = N \frac{\partial m_+}{\partial h} \Big|_{h=0} = \frac{N}{k_B} \left\{ \frac{1}{T_N + T \cosh^2 \left(\frac{T_N}{T} m_0 \right)} \right\}$$

2 Landau diamagnetism of a two-dimensional electron gas

The magnetic properties of a noninteracting electron gas are controlled by two phenomena : the Pauli paramagnetism due to the alignment of the electronic magnetic moments with the applied magnetic field, and the Landau diamagnetism induced by the orbital motion of the electronic charges. In this problem we aim at describing the second of these phenomena, using the one-electron Hamiltonian (in cgs units)

$$H = \frac{1}{2m} \left[\mathbf{p} + \frac{e}{c} \mathbf{A}(\mathbf{r}) \right]^2, \quad (2.1)$$

where $\mathbf{A}(\mathbf{r})$ is the vector potential, $-e$ the electronic charge ($e > 0$), and c the speed of light in vacuum. In Eq. (2.1), m is the (effective) mass of the charge carriers (*i.e.*, the electrons).

In what follows, we consider a homogeneous magnetic field B parallel to the z axis ($B = \partial_x A_y - \partial_y A_x = \text{constant}$), and we assume that electrons are confined to a two-dimensional rectangular surface with area $\mathcal{A} = L_x L_y$, where L_x and L_y are the lateral dimensions of the electron gas in the x and y directions, respectively.

2.1 General results for noninteracting fermions

- (a) Carefully demonstrate that the grand-canonical partition function for noninteracting fermions is given by

$$\Xi = \prod_{\lambda} [1 + e^{-\beta(\epsilon_{\lambda} - \mu)}],$$

where the product runs over quantum states λ with energy ϵ_{λ} . Here, $\beta = 1/k_B T$ with T the temperature and μ is the chemical potential.

$$\begin{aligned} \Xi &= \sum_{(l)} e^{-\beta(\epsilon_l - \mu N_l)} \\ &= \sum_{n_{\lambda_1}=0}^1 \cdots \sum_{n_{\lambda_N}=0}^1 \exp \left[-\beta \left(\sum_{\lambda_1 \cdots \lambda_N} \epsilon_{\lambda} n_{\lambda} - \mu \sum_{\lambda_1 \cdots \lambda_N} n_{\lambda} \right) \right] \\ &= \sum_{n_{\lambda_1}=0}^1 \cdots \sum_{n_{\lambda_N}=0}^1 \prod_{\lambda_1 \cdots \lambda_N} \exp(-\beta(\epsilon_{\lambda} - \mu)n_{\lambda}) \\ &= \prod_{\lambda} \sum_{n_{\lambda}=0}^1 \exp(-\beta(\epsilon_{\lambda} - \mu)n_{\lambda}) \\ &= \prod_{\lambda} [1 + e^{-\beta(\epsilon_{\lambda} - \mu)}] \end{aligned}$$

- (b) Deduce from the previous result that the general expression of the grand potential for noninteracting fermionic particles is given by

$$\Omega = -k_B T \sum_{\lambda} \ln(1 + e^{-\beta(\epsilon_{\lambda} - \mu)}). \quad (2.2)$$

The grand potential is defined as,

$$\Omega = -k_B T \ln \Xi$$

So,

$$\begin{aligned} \Omega &= -k_B T \ln \left\{ \prod_{\lambda} [1 + e^{-\beta(\epsilon_{\lambda} - \mu)}] \right\} \\ &= -k_B T \sum_{\lambda} \ln \{1 + e^{-\beta(\epsilon_{\lambda} - \mu)}\} \end{aligned}$$

2.2 Landau susceptibility

The energy spectrum of the Hamiltonian (2.1) corresponds to the one of a harmonic oscillator with (cyclotron) frequency $\omega_c = eB/mc$ (we assume $B > 0$ from now on) :

$$\epsilon_n = \hbar\omega_c \left(n + \frac{1}{2} \right), \quad n \in \mathbb{N}$$

defining so-called Landau levels. Each Landau level is highly degenerate, with degeneracy factor (including the spin degeneracy)

$$g_n = \rho_0 \hbar\omega_c,$$

where $\rho_0 = m\mathcal{A}/\pi\hbar^2$ is the density of states of the two-dimensional electron gas at zero magnetic field.²

- (a) Give an expression of the grand-potential (2.2) in terms of a summation over Landau levels n and as a function of ρ_0 .

Meaning,

$$\begin{aligned} \Omega &= -k_B T \sum_{\lambda} \ln \{1 + e^{-\beta(\epsilon_{\lambda} - \mu)}\} \\ &= -k_B T \rho_0 \hbar\omega_c \sum_n \ln \{1 + e^{-\beta(\epsilon_n - \mu)}\} \\ &= -k_B T \rho_0 \hbar\omega_c \sum_n \ln \left\{ 1 + e^{-\beta(\hbar\omega_c \{n + \frac{1}{2}\} - \mu)} \right\} \end{aligned}$$

2. Note that the degeneracy factor is in fact independent on n .

(b) The Euler–MacLaurin formula allows one to approximate a discrete summation by the following expression :

$$a \sum_{n=0}^{+\infty} f(a(n + 1/2)) \stackrel{a \ll 1}{\approx} \int_0^{+\infty} dx f(x) + \frac{a^2}{24} f'(0) + \mathcal{O}(a^3),$$

where $f(x)$ is a function that decreases sufficiently fast when $x \rightarrow \infty$, where $f'(x)$ is its derivative with respect to x , and where a is some dimensionless parameter. Use the above formula to show, in the limits $\beta \hbar \omega_c \ll 1$ and $\beta \mu \gg 1$, that

$$\Omega(B) \simeq \Omega(B = 0) + \frac{\rho_0}{24} (\hbar \omega_c)^2,$$

where the expression for $\Omega(B = 0)$ involves an integral not to be calculated.

We saw that,

$$\Omega = -k_B T \rho_0 \hbar \omega_c \sum_n \ln \left\{ 1 + e^{-\beta(\hbar \omega_c \{n + \frac{1}{2}\} - \mu)} \right\}$$

Now, $\beta \hbar \omega_c \ll 1$ and $\beta \mu \gg 1$, meaning,

$$\begin{aligned} \Omega &\approx -k_B T \rho_0 \int_0^{+\infty} \ln \{ 1 + e^{\beta(\mu - \varepsilon)} \} d\varepsilon - k_B T \rho_0 \frac{(\hbar \omega_c)^2}{24} f'(0) \\ &\approx \Omega(B = 0) + \rho_0 \frac{(\hbar \omega_c)^2}{24} \end{aligned}$$

(c) Let us define the Landau susceptibility as

$$\chi_L = -\frac{1}{\mathcal{A}} \lim_{B \rightarrow 0} \frac{\partial^2 \Omega}{\partial B^2}.$$

Show that

$$\chi_L = -\frac{e^2}{12\pi m c^2}$$

We saw the approximation of Ω was,

$$\begin{aligned} \Omega &= \Omega(B = 0) + \rho_0 \frac{(\hbar \omega_c)^2}{24} \\ &= \Omega(B = 0) + \frac{m \mathcal{A} \hbar^2 e^2 B^2}{\pi \hbar^2 24 m^2 c^2} \\ &= \Omega(B = 0) + \frac{\mathcal{A} e^2}{24 \pi m c^2} B^2 \end{aligned}$$

So,

$$\begin{aligned} \chi_L &= -\frac{1}{\mathcal{A}} \lim_{B \rightarrow 0} \frac{\partial^2}{\partial B^2} \left\{ \Omega(B = 0) + \frac{\mathcal{A} e^2}{24 \pi m c^2} B^2 \right\} \\ &= -\frac{e^2}{12 \pi m c^2} \end{aligned}$$