11.3 ff. : Magnetic behavior of an ideal Fermi gas

Consider : gas of non-interacting fermions in the presence of an external magnetic field $\vec{B}$

Comment: We previously looked at system of N magnetic moments

$\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet$

magnetic moments are fixed in space → can point up or down

$$\mathcal{H} = \sum_{i=1}^{N} h_i$$

$\vec{\mu} = \gamma \vec{J}$

gyromagnetic factor

could be $\vec{S}$

Partition function:
(single magnetic moment)

$$e^{\beta\mu B} + e^{-\beta\mu B}$$

$$= 2\cosh(\beta\mu B)$$

$$p_\pm = e^{\pm\beta\mu B}\,\frac{1}{2\cosh(\beta\mu B)}$$

$$\Rightarrow \underset{\text{magnetization}}{\mathcal{M}} = N\langle\mu\rangle = N\mu\tanh\left(\frac{\mu B}{kT}\right)$$

$$\langle\mu\rangle = \mu(p_+ - p_-)$$

In this chapter we are considering a different situation:
- the magnetic moments are <u>not</u> fixed in space
- the fermions instead form a non-interacting gas ($\hat{=}$ are treated as a non-interacting gas) and placed into an external magnetic field

$\mathcal{M}$: Average induced magnetic moment per unit volume of the system along the direction of an external magnetic field B

Note: the text uses H instead of B for B-field

$$\mathcal{M} = \frac{1}{V} \left\langle - \frac{\partial \mathcal{H}}{\partial B} \right\rangle$$

like a "force equation"

derived on next page

$$\Rightarrow \begin{cases} \boxed{\mathcal{M} = kT \left(\frac{\partial}{\partial B} \frac{\log Q_N}{V} \right)_{T,V,N}} & \text{for canonical ensemble} \\[2ex] \mathcal{M} = kT \left(\frac{\partial}{\partial B} \left(\frac{\log \mathcal{Q}}{V} \right) \right)_{T,V,z} & \text{for grand canonical ensemble} \end{cases}$$

z to be eliminated in terms of N

Math detail (derivation of $\mathcal{M} = kT \frac{\partial}{\partial B}\left(V^{-1} \log Q_N\right)$):

Start with:

this eq. defines $\mathcal{M}$

$$\mathcal{M} = \frac{1}{V} \left\langle -\frac{\partial \mathcal{H}}{\partial B} \right\rangle$$

by def.: classical SM, canonical ensemble

$$= \frac{-1}{V} \frac{\int \frac{\partial \mathcal{H}}{\partial B} e^{-\beta \mathcal{H}} d^{3N}p\, d^{3N}q}{\int e^{-\beta\mathcal{H}} d^{3N}p\, d^{3N}q}$$

$$= -\frac{1}{V\beta} \frac{\int \left(\frac{\partial}{\partial B}(\beta\mathcal{H})\right) e^{-\beta \mathcal{H}} d^{3N}p\, d^{3N}q}{\int e^{-\beta\mathcal{H}} d^{3N}p\, d^{3N}q}$$

Now: $\frac{\partial}{\partial B}\left(e^{-\beta\mathcal{H}}\right) = e^{-\beta\mathcal{H}}\left(\frac{\partial}{\partial B}(-\beta\mathcal{H})\right)$ (*)

$\beta = \frac{1}{kT}$

using (*)

$$= \frac{kT}{V} \frac{\int \frac{\partial}{\partial B}\left(e^{-\beta \mathcal{H}}\right) d^{3N}p\, d^{3N}q}{\int e^{-\beta\mathcal{H}} d^{3N}p\, d^{3N}q}$$

Since B is a constant, the derivative can be taken outside the integral

$$= \frac{kT}{V} \underbrace{\frac{\frac{\partial}{\partial B}\int e^{-\beta \mathcal{H}} d^{3N}p\, d^{3N}q}{\int e^{-\beta\mathcal{H}} d^{3N}p\, d^{3N}q}}_{\text{of the form } \frac{\frac{\partial}{\partial B} f}{f}}$$

rewrite as $\frac{\partial}{\partial B} \log f$

$$= \frac{kT}{V} \frac{\partial}{\partial B}\left(\log\left(\underbrace{\int e^{-\beta\mathcal{H}} d^{3N}p\, d^{3N}q}_{Q_N}\right)\right)$$

$$\boxed{\mathcal{M} = kT\left(\frac{\partial}{\partial B}\left(\frac{\log Q_N}{V}\right)\right)_{T,V,N}}$$

We can do the same thing for quantum SM.

χ: magnetic susceptibility per unit volume

$$\chi = \frac{\partial \mathcal{M}}{\partial B}$$

Back to classical system discussed on p. 254:

using

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

from page 254

at high T: $\mathcal{M} = \frac{N\mu^2 B}{kT}$ (use $\tanh x \approx x$)

$$\chi = \frac{N\mu^2}{kT}$$

Curie law

$$\frac{\partial}{\partial B} \tanh\left(\frac{\mu B}{kT}\right) = \frac{\mu}{kT} \underbrace{\operatorname{sech}^2\left(\frac{\mu B}{kT}\right)}_{\to 1 \text{ for } B \to 0}$$

Susceptibility at zero magnetic field at any temperature:

$$\chi_0 = \lim_{B \to 0} \frac{\partial \mathcal{M}}{\partial B} = \frac{N\mu^2}{kT}$$

$\chi > 0$: paramagnet

at low T: "energy dominates" $\to$ smaller E

at higher T: "entropy dominates" $\hookrightarrow$ larger S

system wants to minimize free energy
Helmholtz

$A = U - TS$

In general:

$\chi > 0$: paramagnetism

$\chi < 0$: diamagnetism

We want to treat non-interacting Fermi gas in B-field quantum mechanically:

single-particle energy will be $\frac{\vec{p}^2}{2m} - \vec{\mu} \cdot \vec{B} + \vec{A}$-dep. terms

$\vec{\mu}$: intrinsic magnetic moment of particle

$\vec{A}$: vector potential

give rise to <u>paramagnetism</u> (Sec. 11.6)

give rise to <u>diamagnetism</u> (Sec. 11.3)

due to quantization of the orbits of charged particles in the presence of external magnetic field

might alternatively say:
due to the quantization of the (kinetic) energy of charged particles associated with their motion perpendicular to the direction of the field

In general: we have a "competition" of paramagnetic and diamagnetic tendency

↳ spin-orbit coupling and electron-electron (or fermion-fermion) interactions also need to be taken into account ⇝ they lead to a coupling of the two tendencies

note: in condensed matter systems, spin-orbit coupling is $\vec{p} \cdot \vec{s}$ term

(in atomic and nuclear physics, spin-orbit coupling refers to $\vec{s} \cdot \vec{\ell}$ coupling term → plays a key role in explaining shell structure of nuclei!!!)

Let's start with Pauli paramagnetism (Sec. 11.6)

Single-particle Hamiltonian:

$$\hat{\mathcal{H}} = \frac{\hat{\vec{p}}^2}{2m} - \underbrace{\hat{\vec{\mu}}}_{\text{intrinsic (spin) magnetic moment}} \cdot \hat{\vec{B}}$$

Say, we focus on $\underbrace{\text{spin-}\tfrac{1}{2}}_{\text{specifically, electron}}$ particle for simplicity.

Intrinsic (spin) magnetic moment of electron:

$$\hat{\vec{\mu}} = - g_s \mu_B \frac{1}{\hbar} \hat{\vec{S}}$$

$\uparrow$ magnetic moment is anti-parallel to the spin angular momentum

μ_B : Bohr magneton ($\mu_B = \frac{e\hbar}{2m_e}$) in SI units

g_s : spin g-factor ($g_s \approx 2.002\ 319 \ldots$)

note, g_s is 2 according to Dirac equation $\leadsto$ the small deviation from 2 is due to quantum electrodynamics

numerical value of μ_B:

$$\mu_B = 5.788..10^{-5} \frac{eV}{T}$$

$$1 \text{ Tesla} = 10{,}000 G = 10^4 G$$

$$\text{So: } \mu_B = 5.788 \cdot 10^{-1} \frac{eV}{G}$$

In laboratory settings, B-field strengths up to 1000 G can be generated without too much effort

Let magnetic field lie along +z-axis:

$$\vec{B} = \underbrace{B}_{\text{B is strength of B-field}} \hat{e}_z \Rightarrow -\hat{\vec{\mu}} \cdot \vec{B} = -B \underbrace{\hat{\mu}_z}_{\text{z-component}}$$

$$\frac{1}{\hbar} \hat{S}_z = \frac{1}{2} \hat{\sigma}_z = \frac{1}{2} \left(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow| \right)$$

So: $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \underbrace{\mu_B B \hat{\sigma}_z}_{-\hat{\vec{\mu}}\cdot\vec{B} = \underbrace{-}_{+}\left(-2\mu_B \frac{1}{2}\hat{\sigma}_z\right) B}$

using $g_s = 2$

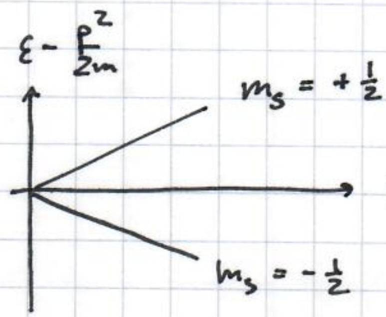
(note: the sign of the second term changed!)

Eigenvalues of single-particle Hamiltonian:

$$\varepsilon = \frac{p^2}{2m} \pm \mu_B B$$

$m_s = \frac{1}{2} \leftarrow$ $+$: spin $\uparrow$ ($\hat{\vec{\mu}}$ anti-parallel to $\hat{\vec{B}}$)

$m_s = -\frac{1}{2} \leftarrow$ $-$: spin $\downarrow$ ($\hat{\vec{\mu}}$ parallel to $\hat{\vec{B}}$)



"alignment parallel to B lowers the energy"

Our goal is now to obtain the susceptibility χ as a function of temperature.

$$E_n = \sum_{\vec{k}} \sum_{m_s} \varepsilon_{\vec{k},m_s} \; n_{\vec{k},m_s}$$

energy of N-particle system

the subscript labels the N-particle energies

occupation number of the single-particle energy level $\varepsilon_{\vec{k},m_s}$

$$= \sum_{\vec{k}} \left[\underbrace{\left(\frac{\hbar^2 \vec{k}^2}{2m} - \mu_B B\right) n^+_{\vec{k}}}_{m_s = -\frac{1}{2}} + \underbrace{\left(\frac{\hbar^2 \vec{k}^2}{2m} + \mu_B B\right) n^-_{\vec{k}}}_{m_s = +\frac{1}{2}} \right]$$

"resolve" the sum over m_s

Superscript +: magnetic moment parallel to field ($m_s = -\frac{1}{2}$)

$n^+_{\vec{k}}$ and $n^-_{\vec{k}}$: 0 or 1

$$\left.\begin{aligned} \sum_{\vec{k}} n^+_{\vec{k}} &= N^+ \\ \sum_{\vec{k}} n^-_{\vec{k}} &= N^- = N - N^+ \end{aligned}\right\}$$

definitions (equations that define N^+ and N^-)

$$\Rightarrow E_n = \sum_{\vec{k}} \left(n^+_{\vec{k}} + n^-_{\vec{k}} \right) \frac{\hbar^2 \vec{k}^2}{2m} - \mu_B B \left(N^+ - N^- \right)$$

Since we have the N-particle energies (at least in principle), we can calculate the partition function.

$$Q_N = \underbrace{\sum_{\{n_k^+\},\{n_k^-\}}{}^{'}}_{} e^{-\beta E_n}$$

the prime on the sum reminds us that we have restrictions

sum over all E_n subject to the conditions / restrictions: $n_k^+, n_k^- = 0$ or 1

$$\sum_k n_k^+ + \sum_k n_k^- = N$$

The evaluation of the sum is a bit tricky due to the fact that we have constraints.

Let's pick one specific N^+ value and sum over all sets $\{n_k^+\}, \{n_k^-\}$ such that

$$\sum_k n_k^+ = N^+ \quad \text{restriction 1}$$

and $\sum_k n_k^- = N - N^+$. restriction 2

Then we sum over all possible N_+ ($N_+ = 0, 1, \ldots, N$).

$$\Rightarrow Q_N = \sum_{N_+=0}^{N} \left[\underline{e^{\beta g_s B (2N^+ - N)}} \left\{ \sum_{\{n_k^+\}}{}'' e^{-\beta \sum_k \frac{\hbar^2 k^2}{2m} n_k^+} \sum_{\{n_k^-\}}{}''' e^{-\beta \sum_k \frac{\hbar^2 k^2}{2m} n_k^-} \right\} \right]$$

this is "just" $e^{\beta g_s B (N^+ - N^-)}$

subject to restriction 1

subject to restriction 2

Define: $$Q_N^{(0)} = \underbrace{\sum_{\sum n_{\vec{k}} = N}}_{} e^{-\beta \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} n_{\vec{k}}} = e^{-\beta A_0(N)}$$

earlier, this type of sum was written as $\sum_{\{n_{\vec{k}}\}}'$

this is the partition fct. of the spinless ideal Fermi gas consisting of N particles

$$\Rightarrow Q_N = e^{-\beta \mu_B B N} \sum_{N_+=0}^{N} e^{2\beta\mu_B B N_+} Q_{N_+}^{(0)} \underbrace{Q_{N_-}^{(0)}}_{\text{or } Q_{N-N_+}^{(0)}}$$

taking logarithm $\Rightarrow$
$$\frac{1}{N}\log Q_N = -\beta\mu_B B + \underbrace{\frac{1}{N}\log\Bigg(\underbrace{\sum_{N_+=0}^{N} e^{2\beta\mu_B B N_+ - \beta A_0(N_+) - \beta A_0(N_-)}}_{N+1 \text{ positive terms}}\Bigg)}_{\log(\text{largest term in sum}) + \frac{1}{N}\log N \text{ type terms}}$$

correction

To find largest contribution: look at exponent and take derivative with respect to N_+

we're forcing this to be zero

$$\rightarrow \underbrace{2\mu_B B - \underbrace{\frac{\partial A_0(N_+)}{\partial N_+}}_{\mu_0(N_+)} - \underbrace{\frac{\partial A_0(N-N_+)}{\partial N_+}}_{-\mu_0(N-N_+)}}_{} = 0$$

NR:

$$\frac{\partial A_0(N-N_+)}{\partial N_+} = \frac{\partial A_0(N-N_+)}{\partial N_-}\underbrace{\frac{\partial N_-}{\partial N_+}}_{-1} = -\frac{\partial A_0(N-N_+)}{\partial N_-}$$

this equation yields $\bar{N}_+$

(the $\bar{N}_+$ found in this way gives the largest contribution to the sum inside the logarithm)

$$\rightarrow 2\mu_B B = \mu_0(\bar{N}_+) - \mu_0(N - \bar{N}_+)$$

recall, these are chemical potentials of our fictitious spinless Fermi gas

While not overly explicit, we have found a general solution!

More detail on: How to get $\mathcal{M} = \frac{1}{V}\mu_B N r$?

By definition: $\mathcal{M} = kT\left(\frac{\partial}{\partial B}\left(\frac{\log Q_N}{V}\right)\right)_{N,T,V}$ see page 255

What do we have for $\log Q_N$? Look at bottom of page 264:

$\log Q_N = -\beta N \mu_B B + \log\left(\text{"(N+1) positive terms"}\right)$

We found that the largest contribution was given for $\underbrace{2\mu_B B}_{\text{result given on page 266, (*)}} = \mu_0\left(\frac{1+r}{2}N\right) - \mu_0\left(\frac{1-r}{2}N\right)$

$$\Rightarrow \log\left(\sum_{N_+=0}^{N} e^{2\beta\mu_B B N_+ - \beta A_0(N_+) - \beta A_0(N_-)}\right)$$

$$\xrightarrow[\text{one term}]{\text{keeping just}} 2\beta\mu_B B\bar{N}_+ - \beta A_0(\bar{N}_+) - \beta A_0(N-\bar{N}_+)$$

$$\Rightarrow \log Q_N \approx \beta\mu_B B(\underbrace{2\bar{N}_+ - N}_{Nr}) - \underbrace{\beta A_0\left(\frac{r+1}{2}N\right) - \beta A_0\left(\frac{1-r}{2}N\right)}_{}$$

these are the Helmholtz free energies of the fictitious spinless Fermi gas

$\rightarrow$ these terms are independent of B !!!

$$\Rightarrow \mathcal{M} = kT\left(\frac{\partial}{\partial B}\left(\frac{\log Q_N}{V}\right)\right)_{N,T,V} = \frac{1}{V}\mu_B N r \underset{\text{by def. of } r}{=} \frac{1}{V}\mu_B(\bar{N}_+ - \bar{N}_-)$$

Let's define : $\underbrace{\bar{N}_+ - \bar{N}_-}_{2\bar{N}_+ - N} = N r$, where $0 \le r \le 1$.

$2\bar{N}_+ = N(r+1) \Rightarrow \boxed{\bar{N}_+ = \frac{1+r}{2} N}$

Using r, we can write:

$$2\mu_B B = \mu_0 \Big(\underbrace{\tfrac{1+r}{2} N}_{\bar{N}_+} \Big) - \mu_0 \Big(\underbrace{\tfrac{1-r}{2} N}_{N - \bar{N}_+} \Big) \quad (*)$$

on previous page: $\bar{N}_+$

$B=0$ implies $\mu_0\left(\frac{1+r}{2}N\right) = \mu\left(\frac{1-r}{2}N\right) \Rightarrow r=0$

if $B \to 0 \Rightarrow r \to 0$ and $\bar{N}_+ \to \bar{N}_-$

So, we can think of small r as corresponding to small B

Note : $\boxed{V\mathcal{M} = \mu_B (\bar{N}_+ - \bar{N}_-) = \mu_B N r}$

see next page for derivation of $V\mathcal{M} = \mu_B N r$

to get small-r expression,

Taylor expand r.h.s. of (*)

around $r = 0$ (leading terms cancel, first order terms give $\frac{1}{2} + \frac{1}{2} = 1$):

$$\rightsquigarrow 2\mu_B B \approx \left.\frac{\partial \mu_0 (xN)}{\partial x}\right|_{x=\frac{1}{2}} r$$

$$\Rightarrow r = \frac{2\mu_B B}{\left.\frac{\partial \mu_0(xN)}{\partial x}\right|_{x=\frac{1}{2}}}$$

susceptibility per unit volume $\Rightarrow \chi = \frac{\partial \mathcal{M}}{\partial B}$

$$= \frac{\partial}{\partial B}\left(\frac{2\mu_B^2 B N}{V \left.\frac{\partial \mu_0(xN)}{\partial x}\right|_{x=\frac{1}{2}}} \right)$$

$$= \frac{1}{V} \frac{2\mu_B^2 N}{\left.\frac{\partial \mu_0(xN)}{\partial x}\right|_{x=\frac{1}{2}}} = \frac{2n\mu_B^2}{\left.\frac{\partial \mu_0(xN)}{\partial x}\right|_{x=\frac{1}{2}}}$$

density $n = \frac{N}{V}$

From $\mathcal{M} = \frac{1}{V}\mu_B N r$

we get

$$\mathcal{M} = \frac{1}{V}\mu_B^2 N \frac{2B}{\left.\frac{\partial \mu_0(xN)}{\partial x}\right|_{x=\frac{1}{2}}}$$

using result for r

What is $\mu_0(xN)$?

$$\mu_0(xN) = \left(\frac{3xN}{4\pi V}\right)^{2/3} \frac{h^2}{2m}$$

(this is h – not $\hbar$!)

So: χ is positive $\rightsquigarrow$ paramagnetic effect !!!

Next : Landau diamagnetism (see Sec. 11.3)

Note: the discussion here is fairly brief → I want to bring the idea across.

orbital motion feels B field

e positive (charge of electron $-e$)

Classically : $\mathcal{H}_{cl} = \frac{1}{2m}\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2$ (for electron)

single-particle Hamiltonian

vector potential

Let's choose the following gauge : $A_x = -By$, $A_y = 0$, $A_z = 0$ — magnetic field along z-direction

$$\Rightarrow \mathcal{H}_{cl} = \frac{1}{2m}\left(p_x - \frac{e}{c}By\right)^2 + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$$

Now quantize :

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{p}_x - \frac{e}{c}B\hat{y}\right)^2 + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m}$$

Strategy : • Solve single-particle Hamiltonian
• Construct grand partition function
• Calculate susceptibility

Make educated guess:

$$\psi(x,y,z) = \underbrace{e^{i(k_x x + k_z z)}}_{\text{plane waves in } x \text{ and } z} f(y)$$

We find: $\left[\frac{\hat{p}_y^2}{2m} + \frac{1}{2} m \omega_0^2 (y-y_0)^2\right] f(y) = \bar{\mathcal{E}} f(y)$

where $\bar{\mathcal{E}} = \mathcal{E} - \frac{\hbar^2 k_z^2}{2m}$

$\omega_0 = \frac{eB}{mc}$

cyclotron frequency

$y_0 = \frac{\hbar c}{eB} k_x$

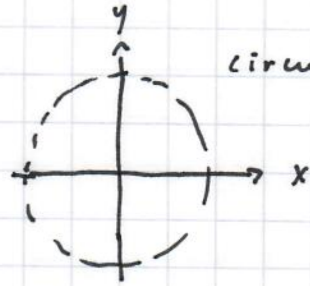
$$\Rightarrow \mathcal{E} = \underbrace{\frac{e\hbar B}{mc}}_{\hbar\omega_0} \left(j + \frac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m}$$

$j = 0, 1, 2, \ldots$

$\rightarrow$ $\underbrace{\text{no dependence on } k_x}_{\text{yes and no...}}$

there is a somewhat hidden dependence due to degeneracy of energy levels

Classical trajectory:



circular motion $\rightsquigarrow$ angular velocity ω_0

helical path (constant linear velocity)

Quantum mechanical energy level structure:

xy-plane: quantization in units of $\hbar\omega_0$

recall $y_0 = \frac{\hbar c}{eB} k_x$ $\rightsquigarrow$ allowed values of k_x:

$$k_x = \frac{2\pi}{L} n_x \; ; \; n_x = 0, \pm 1, \pm 2, \ldots$$

Assume system is inside a cube of size L^3

$\Rightarrow$ y_0 must lie between 0 and L

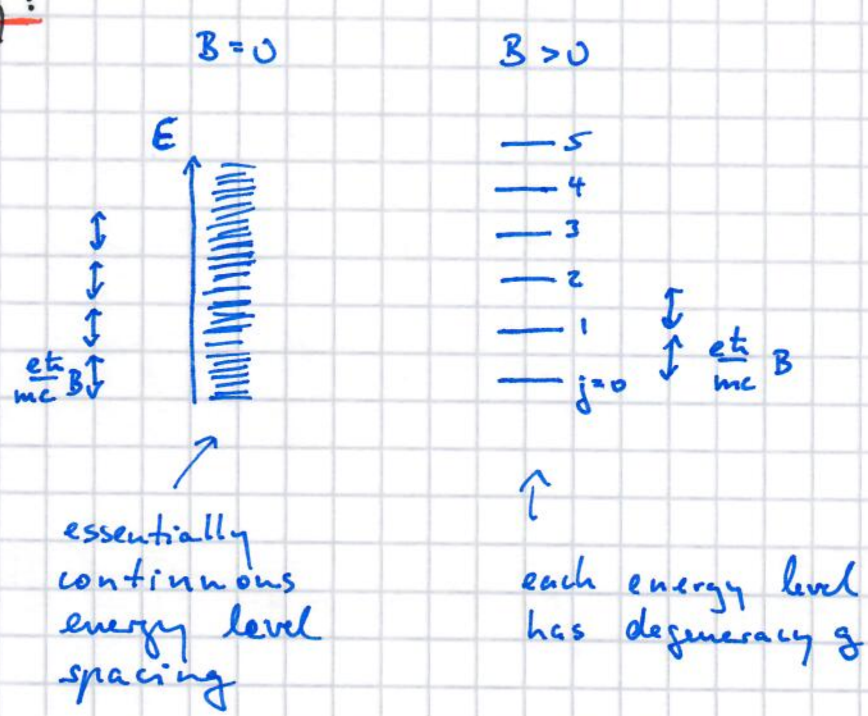
$\Rightarrow$ $k_x = \frac{eB}{\hbar c} y_0$ must lie between 0 and $\frac{eB}{\hbar c} L$

$\Rightarrow$ $n_x \geq 0$ and $n_x \leq \frac{L k_x}{2\pi} \leq \frac{eB}{hc} L^2$

$g = \frac{eB}{hc} L^2$ is degeneracy of each Landau level

The degeneracy or multiplicity factor g is a quantum mechanical measure of the freedom available to the particle (for the center of its orbit to be located anywhere in the area L^2).

Pictorially:



Grand partition function:

$$\log \mathcal{Q} = \sum_{\varepsilon} \log\left(1 + z e^{-\beta\varepsilon}\right)$$

sum over all single-particle states

equilibrium number $\bar{N}$ of particles:

$$\bar{N} = \left(z \frac{\partial}{\partial z} \log \mathcal{Q} \right)_{B,V,T}$$

magnetic moment:

$$\mathcal{M} = kT \left(\frac{\partial}{\partial B} \left(\frac{\log \mathcal{Q}}{V} \right) \right)_{T,V,z}$$

After a bit of work: $\left(\text{let } x = \beta \frac{e\hbar}{4\pi mc} B = \beta \mu_B B \right)$

high temperature limit: $z \ll 1$

$$\bar{N} = \frac{zV}{\lambda^3} \frac{x}{\sinh x}$$

$$\mathcal{M} = \frac{z}{\lambda^3} \frac{eh}{4\pi mc} \left(\frac{1}{\sinh x} - \frac{x \cosh x}{\sinh^2 x} \right)$$

$$\Rightarrow \mathcal{M} = -\frac{\bar{N}}{V} \frac{eh}{4\pi mc} \left(\coth x - \frac{1}{x} \right)$$

$$= -\frac{\bar{N}}{V} \mu_B \underbrace{\left(\coth x - \frac{1}{x} \right)}_{\text{Langevin fct.}}$$

$\mu_B = \frac{e\hbar}{2mc}$ in CGS units

$$\chi = -\frac{1}{3kTv} \mu_B^2$$

diamagnetism

$\rightarrow \frac{1}{T}$ behavior (as in Curie's law)