Stat Mech. Tutorial 3-2

De Haas-Van Alphen effect

We considered $\mu_B B < T \ll \mu \; (= \varepsilon_F)$ Let us now consider

$T \lesssim \mu_B B \ll \mu$ (strong fields)

Will show that the magnetization oscillates.

Simple model

$T = 0$, ignore the z direction of motion, ignore spin: $\pm \mu_B B$.

Area L^2.

For $T=0$ the free energy: $F = E_0$ (ground state energy of the system)

$$\Rightarrow \quad M = -\frac{\partial E_0}{\partial B}$$

We saw $\varepsilon_j = 2\mu_B B (j + \frac{1}{2})$

$$g = \frac{NB}{B_0} \quad \text{where} \quad B_0 \equiv \frac{N}{L^2}\frac{hc}{2e} = n\frac{hc}{2e}$$

n: no. electrons per area.

For $B > B_0$ the lowest state can hold all of the electrons.

Then $\frac{E_0}{N} = \mu_B B$, $M = -\mu_B N$.

As we decrease the field to $\frac{B}{B_0} < 1 \rightarrow$ occupy higher levels.

Suppose B: $j+1$ lowest levels filled - up to level "j"

$(j+2)$th partialy filled (the one with $j+1 = k$)

rest empty

$$\Rightarrow \quad \underbrace{g(j+1)}_{j+1 \text{ levels filled}} < N < \underbrace{g(j+2)}_{\text{less than } j+2 \text{ filled}}$$

$$\Rightarrow \quad \frac{1}{j+2} < \frac{B}{B_0} < \frac{1}{j+1} \qquad \left(g = \frac{NB}{B_0}\right)$$

Then the energy is:

$$\frac{E_0}{N} = \frac{1}{N}\Big(\underbrace{g\sum_{i=0}^{j}\varepsilon_i}_{\text{filled levels}} + \underbrace{[N-(j+1)g]}_{\substack{\text{no. of electrons}\\ \text{left for}\\ \text{level } k=j+1}}\varepsilon_{j+1}\Big) = \mu_B B\Big[2j+3+\sum_{k=0}^{j}(2k+1)\frac{B}{B_0} - \frac{B}{B_0}(j+1)(2j+3)\Big]$$

$$\boxed{\varepsilon_{j+1} = \mu_B B(2j+3)}$$

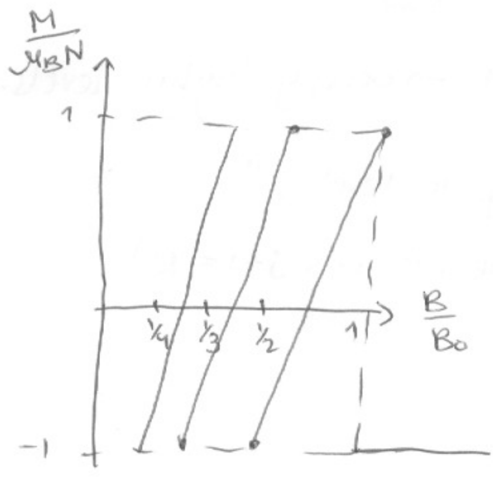
$$\sum_{k=0}^{j}(2k+1) = \frac{(1+2j+1)(j+1)}{2} = (j+1)^2$$

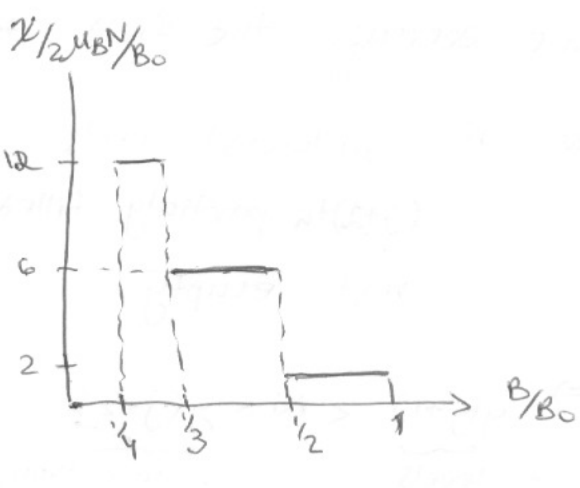
$$(j+1)^2 - (j+1)(2j+3) = (j+1)(-j-2)$$

$$\frac{E_0}{N} = \mu_B B\left(2j+3 - \frac{B}{B_0}(j+1)(j+2)\right) \qquad \frac{1}{j+2} < \frac{B}{B_0} < \frac{1}{j+1}$$

$$M = \begin{cases} -\mu_B N & B > B_0 \\ \mu_B N\left[2\frac{B}{B_0}(j+1)(j+2) - 2j - 3\right] & \frac{1}{j+2} < \frac{B}{B_0} < \frac{1}{j+1} \end{cases}$$

$$\chi = \begin{cases} 0 & B > B_0 \\ \frac{2\mu_B N}{B_0}(j+1)(j+2) & \frac{1}{j+2} < \frac{B}{B_0} < \frac{1}{j+1} \end{cases}$$





For $T \neq 0$ we expect this to smoothen up.

Let us make the full calculation with z, $T \neq 0$.

$$T \lesssim \mu_B B \ll \mu$$

Now we can't find corrections from orbital and spin separately.

The energy levels:

$$\varepsilon_n = \frac{p_z^2}{2m} + (2n+1)\mu_B B \pm \mu_B B$$

$\Rightarrow$ can use $\varepsilon = \frac{p_z^2}{2m} + 2n\mu_B B$

with degeneracy $2g$ for $n = 1, 2, \ldots$ and g for $n = 0$.

We can therefore write

$$\Omega = 2\mu_B B \left[\frac{1}{2} f(\mu) + \sum_{n=1}^{\infty} f(\mu - 2\mu_B B n) \right]$$

$$f(\mu) = -\frac{TmV}{2\pi^2\hbar^3} \int_{-\infty}^{\infty} \log\left[1 + \exp\left[\frac{\mu}{T} - \frac{p_z^2}{2m}\right]\right] dp_z$$

again use form $\varepsilon - \mu$, degeneracy.

Interested in oscillatory part of the sum.

Poisson formula:

$$\sum_{n=-\infty}^{\infty} \delta(x-n) = \sum_{k=-\infty}^{\infty} e^{2\pi i k x}$$

← expansion in fourier series

$$\left(C_n = \int_{x_0}^{x_0+1} \sum_{k=-\infty}^{\infty} \delta(t-n) e^{-i2\pi n t} \, dt = \int_{-1/2}^{1/2} \sum_{n=-\infty}^{\infty} \delta(t-n) e^{-i2\pi n t} \, dt = 1 \right)$$

fourier coefficient

over a period $=1$

multiply by $F(x)$ & integrate from 0 to ∞

$\int_0^{\infty} \delta(x) dx = \frac{1}{2}$

$$\Rightarrow \frac{1}{2} F(0) + \sum_{n=1}^{\infty} F(n) = \int_0^{\infty} F(x) dx + 2 \operatorname{Re} \sum_{k=1}^{\infty} \int_0^{\infty} F(x) e^{2\pi i k x} dx$$

using $F(n) = f(\mu - 2\mu_B B n)$ and recalling that

$$2\mu_B B \int_0^\infty f(\mu - 2\mu_B B x)\, dx = \Omega_0(\mu)$$

we get:

$$\Omega = \Omega_0(\mu) + \frac{T m V}{\pi^2 \hbar^3} \,\mathrm{Re} \sum_{k=1}^\infty I_k$$

$$I_k = -2\mu_B B \int_{-\infty}^{\infty} dp_z \int_0^\infty \log\left[1 + \exp\left[\frac{\mu}{T} - \frac{p_z^2}{2mT} - \frac{2x\mu_B B}{T}\right]\right] e^{2\pi i k x}\, dx$$

Change variables: $x \to \varepsilon = \frac{p_z^2}{2m} + 2x\mu_B B$

$$dx = \frac{d\varepsilon}{2\mu_B B}$$

$$I_k = -\int_{-\infty}^{\infty} dp_z \int_{\frac{p_z^2}{2m}}^{\infty} d\varepsilon \log\left[1 + \exp\left[\frac{\mu - \varepsilon}{T}\right]\right] e^{\frac{\pi i k \varepsilon}{\mu_B B}} \exp\left[\frac{i\pi k p_z^2}{2m\mu_B B}\right]$$

Integral p_z dominated by $\frac{p_z^2}{2m} \sim \mu_B B$

Will see later that the oscill. part comes from $\varepsilon \sim \mu$.

Since $\mu \gg \mu_B B$ can replace lower limit by 0

(subdominant contr.)

$\Rightarrow$ The integrals decouple.

p_z integral:

use: $\int_{-\infty}^{\infty} e^{-i\alpha p^2}\, dp = e^{-i\pi/4}\sqrt{\frac{\pi}{\alpha}}$ (replacing $p^2 = e^{-i\pi/2} u$ rotating contour of integration to complex p, u real $\to$ Gaussian)

$\alpha = \frac{\pi k}{2m\mu_B B}$

$$\Rightarrow \tilde{I}_k = -e^{-i\pi/4}\sqrt{\frac{2m\mu_B B}{k}} \int_0^\infty \log\left[1 + e^{(\mu - \varepsilon)/T}\right] e^{\frac{i\pi k \varepsilon}{\mu_B B}}\, d\varepsilon$$

only integral:

Integrate twice by parts and ignore non oscillatory terms:

$$① = \frac{\mu_B B}{T i\pi k} \int_0^\infty \frac{e^{(\mu-\varepsilon)/T}}{1+\exp[(\mu-\varepsilon)/T]} \exp\left[\frac{i\pi k \varepsilon}{\mu_B B}\right] = \frac{\mu_B B}{i\pi k T} \int_0^\infty \frac{1}{e^{(\varepsilon-\mu)/T}+1} e^{\frac{i\pi k\varepsilon}{\mu_B B}} d\varepsilon$$

$$② = -\left(\frac{\mu_B B}{\pi k T}\right)^2 \int_0^\infty \frac{e^{\frac{(\varepsilon-\mu)}{T}}}{\left(e^{\frac{(\varepsilon-\mu)}{T}}+1\right)^2} e^{\frac{i\pi k \varepsilon}{\mu_B B}} d\varepsilon$$

change variables: $\xi = \frac{\varepsilon-\mu}{T} \to \varepsilon = T\xi + \mu$

$$= -\left(\frac{\mu_B B}{\pi k}\right)^2 \frac{1}{T} \int_{-\mu/T}^\infty \frac{e^\xi}{(e^\xi+1)^2} e^{\frac{iT\pi k \xi}{\mu_B B}} e^{i\frac{\mu \pi k}{\mu_B B}}$$

$$\tilde{I}_k = \frac{\sqrt{2m}(\mu_B B)^{5/2}}{T\pi^2 k^{5/2}} \exp\left[\frac{i\pi k \mu}{\mu_B B} - \frac{i\pi}{4}\right] \int_{\underset{\substack{\uparrow \\ \mu \gg T}}{-\infty}}^\infty \frac{e^\xi}{(e^\xi+1)^2} \exp\left[\frac{iT\pi k}{\mu_B B}\right]$$

Indeed,
when $\mu_B B \gtrsim T$ the range $\xi \sim 1$ dominates the integral
i.e $\varepsilon - \mu \sim T$ ε near μ.

$$\int_{-\infty}^\infty \frac{e^\xi}{(e^\xi+1)^2} e^{i\alpha\xi} d\xi = \frac{\pi\alpha}{\sinh \pi\alpha}$$

(using $u = \frac{1}{e^\xi+1}$ get $\int_0^1 (1-u)^{i\alpha} u^{-i\alpha} du = \Gamma(1+i\alpha)\Gamma(1-i\alpha)\Gamma(2)$

beta function

$\Gamma(1-z)\Gamma(1+z) = \frac{\pi z}{\sin \pi z}$)

$$\Omega_{osc} = \frac{\sqrt{2}(m\mu_B B)^{3/2} TV}{\pi^2 \hbar^3} \sum_{k=1}^\infty \frac{\cos\left(\frac{\pi\mu k}{\mu_B B} - \frac{1}{4}\pi\right)}{k^{3/2} \sinh\left(\frac{\pi^2 k T}{\mu_B B}\right)}$$

the sinh has an argument that is small and the cos is large - fast oscillating. Can dif only cos

$$\tilde{M} = -\frac{\sqrt{2}\mu_B\, m^{3/2}\mu T V}{\pi\hbar^3\sqrt{B}} \sum_{k=1}^{\infty} \frac{\sin\left(\frac{\pi\mu k}{\mu_B B} - \frac{\pi}{4}\right)}{\sqrt{k}\,\sinh\left(\pi^2 k T/\mu_B B\right)}$$

$T \ll B \ll \mu$

it's period in $\frac{1}{B}$ is constant: $\Delta\left(\frac{1}{B}\right) = \frac{2\mu_B}{\mu}$

ind. of temp.

For $\mu_B B \sim T$ $\quad |\tilde{M}| \sim V\mu\sqrt{B}\,(m\mu_B)^{3/2}\hbar^{-3}$

(use $\sinh^{-1}(\,) \sim \left(\left(\frac{\mu_B B}{\pi^2 k T}\right)^{-1}\right)$ (large B)

the monotonic part from previous calc.

$$\bar{M} \sim V\mu^{1/2} B\, m^{3/2}\mu_B^2\,\hbar^{-3}$$

$$\frac{\tilde{M}}{\bar{M}} \sim \left(\frac{\mu}{\mu_B B}\right)^{1/2}$$ → amplitude of oscillating part large compared to the monotonic.

For $\mu_B B \ll T$ the amplitude is exponentially small

$\sim \exp\left[-\frac{\pi^2 T}{\mu_B B}\right]$ ← non analytic function

$e^{-1/z}$ ← that's why E-M formula can't give these oscill.

Stat Mech - Tutorial 3 - 1

Ideal Quantum Gasses - recipe

1. Find energies and degeneracies (eigenvalues..)
2. Work in GC ensemble

Others aren't wrong, just difficult.

In GC z, V, T are given

Usually know N not $z \to$ need an equation relating them.

3. F.D or B.E distribution

$$n_i = \#\text{ of fermions/bosons in quantum state } i = \frac{1}{z^{-1}e^{\beta\varepsilon_i} \pm 1}$$ (upper sign - fermions)

$\Rightarrow$ (a) $N = \sum_i \frac{1}{z^{-1}e^{\beta\varepsilon_i} \pm 1} = \sum_i n_i$

(b) $E = \sum_i \varepsilon_i n_i$

(c) $-PV = \Omega = \mp T \sum_i \ln(1 \pm z e^{-\beta\varepsilon_i})$

Note: (a)-(c) have difficult sums, whenever possible pass

$\Sigma \to \int$. (Euler-Maclaurin formula etc.)

Magnetic properties of materials - (Gas of Electrons)

Two phenomena we will talk about

(Ferromagnetizm - interactions of spins later)

Paramagnetism - particles with spin align in the direction of magnetic field (intrinsic magnetic moment)

<u>Diamagnetism</u> - Charged particles moving in magnetic field - loops of current - magnetic moment.

Expect the direction of rotation so that resultant magnetic field opposit to external. (Lorentz force / Le-chatelier principle)

Consider the classical motion of free electrons in magnetic field.

* Move in circles perpendicular to $\vec{B}$

* Radius: $r = \frac{mv}{|e| B}$ v - velocity perp. to field

$\left(\frac{mv^2}{r} = evB\right)$

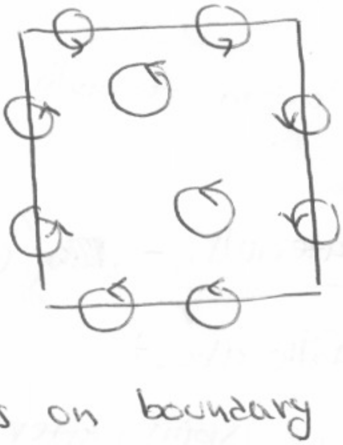
* Magnetic moment $\vec{M} = -\frac{|e|}{2} \vec{r} \times \vec{v}$

$$M = \frac{mv^2}{2B}$$

Doesn't make sense! ∞ for $B = 0$.

Problem: didn't consider boundaries!

Indeed:



$\otimes$ B inside

few electrons on boundary but large loop in opposite direction

$M = I A$ ← area of loop
↑ current

→ can cancel total magnetic moment.

Eeasier to use partition function, only then calculate magnetic moment.

$$M = -\frac{\partial F}{\partial B}$$

$$Z = e^{-\beta F} = \int e^{-\beta H(p,r)} d^3r\, d^3p$$

H- Hamiltonian

$H = V(r) + \frac{1}{2m}(p - eA)^2$ A - vector potential

Change variables: $q = p - eA \rightarrow$ no more A in $Z \rightarrow \frac{\partial}{\partial B} Z = 0$

No classical diamagnetism! (Bohr-van Leuwen theorem)

<u>Magnetism of an electron gas for weak fields</u> - (Quantum)

Calculate magnetic susceptibilities (paramagnetic + diamagnetic) for degenerate electron gas ($T \ll \varepsilon_F$) and weak magnetic field ($\mu_B B \ll T$, $\mu_B = \frac{|e|\hbar}{2mc}$ ~~Bohr~~ Bohr magneton)

Recall that for $T \gg \varepsilon_F$ $\chi_{para} = N\frac{\mu_B^2}{VT}$ Curie's law.

<u>GC ensemble</u>: $M = -\left(\frac{\partial \Omega}{\partial B}\right)_{T,V,\mu}$

Have contribution from spins to energy: $\pm \mu_B B$ and from orbital energy levels. Treat separately.

Since $\Omega = -T\sum_i \ln\left(1 + e^{\beta(\mu - \varepsilon_i)}\right)$

can write

spin degeneracy in $\tilde{\Omega}$

$$\Omega(\mu) = \frac{1}{2}\tilde{\Omega}(\mu + \mu_B B) + \frac{1}{2}\tilde{\Omega}(\mu - \mu_B B)$$

using the form $\mu - \varepsilon_i$ where $\tilde{\Omega}$ is the potential without the splitting $\pm\mu_B B$.

Weak fields - want to expand Ω in powers of B.

Two ~~condition~~ contributions:

$$\Omega(\mu) = \Omega_0(\mu) + \text{leading correction from spin} + \text{leading correction orbital}$$

potential with $B=0$

expand $\frac{1}{2}\Omega_0(\mu+\mu_B B)+\frac{1}{2}\Omega_0(\mu-\mu_B B)$

expand $\tilde{\Omega}(\mu)$

Start with Paramagnetism (due to spins):

$$\frac{1}{2}\Omega_0(\mu+\mu_B B)+\frac{1}{2}\Omega_0(\mu-\mu_B B) \approx \Omega_0(\mu) + \frac{1}{2}\mu_B B\frac{\partial\Omega_0}{\partial\mu} - \frac{1}{2}\mu_B B\frac{\partial\Omega_0}{\partial\mu}$$
$$+\frac{1}{4}(\mu_B B)^2\frac{\partial^2\Omega_0}{\partial\mu^2} + \frac{1}{4}(\mu_B B)^2\frac{\partial^2\Omega_0}{\partial\mu^2} = \Omega_0(\mu) + \frac{(\mu_B B)^2}{2}\frac{\partial^2\Omega_0}{\partial\mu^2}$$

$$M_{para} = -\frac{\partial\Omega}{\partial B} = -\mu_B^2 B\frac{\partial^2\Omega_0}{\partial\mu^2} \quad ; \quad \frac{\partial\Omega_0}{\partial\mu} = -N$$

$$\chi_{para} = \frac{1}{V}\frac{\partial M}{\partial B} = -\frac{\mu_B^2}{V}\frac{\partial^2\Omega_0}{\partial\mu^2} = \frac{\mu_B^2}{V}\frac{\partial N}{\partial\mu}$$

Assuming the gas is completely degenerate ($\mu=\varepsilon_F$, neglecting correction $\frac{T}{\varepsilon_F}$)

$$N = V\frac{(2m\mu)^{3/2}}{3\pi^2\hbar^3} = \frac{p_F^3}{V\pi^2\hbar^3}\ , \qquad \frac{\partial N}{\partial\mu} = \frac{V}{2}\frac{\sqrt{2m\mu}\,2m}{\pi^2\hbar^3}$$

$$\chi_{para} = \frac{\mu_B^2(2m)^{3/2}\sqrt{\mu}}{2\pi^2\hbar^3} = \frac{\mu_B^2 p_F m}{\pi^2\hbar^3}$$

$\rightarrow$ Independent of temperature!

Breaks Curie's law.

Diamagnetic contribution

Need to expand $\tilde{\Omega}(\mu)$ using the quantum expression for energy.

potential without spin

Energy levels: $\varepsilon = \frac{p_z^2}{2m} + (2n+1)\mu_B B$ harmonic motion in plane

Degeneracy: $g = \left(\frac{eB}{hc}\right) L^2$ L - size of box

(comes from a choice to place the y_0 in the plane)

Degeneracy including z motion: no. of levels in dp_z interval:

$$p_z = \frac{2\pi\hbar n_z}{L} \qquad \left(\frac{eB}{hc}\right) L^2 \, dn_z = V \frac{eB}{(2\pi\hbar)^2 c} dp_z$$

Assume thermal wavelength $\lambda_T = \left(\frac{2\pi\hbar^2}{mT}\right)^{1/2} \ll L$ $\left(T \gg \# \frac{1}{L} \right)$

so we can treat p_z as continuous.

$$\tilde{\Omega} = \underset{\uparrow \text{ spin}}{2}\mu_B B \sum_{n=0}^{\infty} f(\mu - (2n+1)\mu_B B)$$

$$f(\mu) = -\frac{TmV}{2\pi^2\hbar^3} \int_{-\infty}^{\infty} \log\left[1 + \exp\left[\mu - \frac{p_z^2}{2m}\right]\right] dp_z$$

Used degeneracy and μ_B to write in this form (and $\varepsilon - \mu$).

Approximate sum by integral (small $\mu_B B$ compared to T), need first correction.

Massage Euler-Maclaurin formula:

$$\sum_{n=0}^{\infty} F(a+n) \simeq \int_a^{\infty} F(x)\,dx + \frac{1}{2}F(a) - \frac{1}{12}F'(a)$$

* take $a=\frac{1}{2}$

* in segment $0\le x\le \frac{1}{2}$ $\quad F(x)\simeq F(0)+xF'(0)$ (Taylor)

* Use $\frac{1}{2}F(\frac{1}{2})\approx \frac{1}{2}F(0)+\frac{1}{4}F'(0)=\int_0^{1/2}F(x)dx+\frac{1}{8}F'(0)$

* $\int_0^{1/2}F(x)dx \approx \int_0^{1/2}(F(0)+xF'(0))dx \simeq \frac{1}{2}F(0)+\frac{1}{8}F'(0)$

* $\frac{1}{12}F'(\frac{1}{2})\approx\frac{1}{12}F'(0)$

$$\Rightarrow \quad \sum_{n=0}^{\infty}F(n+\tfrac{1}{2})\simeq\int_0^{\infty}F(x)dx+\left(\tfrac{1}{8}-\tfrac{1}{12}\right)F'(0)=\int_0^{\infty}F(x)dx+\tfrac{1}{24}F'(0)$$

$$\tilde{\Omega}=2\mu_B B\sum_{n=0}^{\infty}f(\mu-(n+\tfrac{1}{2})2\mu_B B)\simeq 2\mu_B B\int_0^{\infty}dx\, f(\mu-2\mu_B Bx)$$

$$+\frac{2\mu_B B}{24}\left[\frac{\partial f(\mu-2n\mu_B B)}{\partial n}\right]_{n=0}=\int_{-\infty}^{\mu}dy\, f(y)-\frac{(2\mu_B B)^2}{24}\frac{\partial f(\mu)}{\partial\mu}$$

$y=\mu-2\mu_B Bx$

The first term is $\Omega_0(\mu)$, $\quad \frac{\partial\Omega_0(\mu)}{\partial\mu}=f(\mu)$

$$\tilde{\Omega}=\Omega_0(\mu)-\frac{1}{6}\mu_B^2B^2\frac{\partial^2\Omega_0(\mu)}{\partial\mu^2}$$

$$\Rightarrow\quad M=\frac{1}{3}\mu_B^2B^2\frac{\partial^2\Omega_0(\mu)}{\partial\mu^2}$$

$$\chi_{dia}=\frac{1}{3}\frac{\mu_B^2}{V}\frac{\partial^2\Omega_0(\mu)}{\partial\mu^2}=-\frac{1}{3}\frac{\mu_B^2}{V}\frac{\partial N}{\partial\mu}=-\frac{1}{3}\chi_{para}$$

$$\chi_{tot}=\frac{2}{3}\chi_{para}$$

This holds also for $T\gg\varepsilon_F$ (used this only to express $\frac{\partial N}{\partial\mu}$).