Magnetic properties of Free Electron Gas

In the presence of an applied magnetic field $\mathbf{H}$, the electron gas will develop a net magnetization via two effects:

1) The intrinsic spins of the electrons anti-align with $\mathbf{H}$ ⇒ magnetic moments align with $\mathbf{H}$ ⇒ paramagnetic effect
   \[ \text{Pauli Paramagnetism} \]

2) The electrons move in closed orbits ⇒ circulating currents ⇒ magnetic moments anti-aligned with $\mathbf{H}$ ⇒ diamagnetic effect
   \[ \text{Landau diamagnetism} \]

We consider just Pauli Paramagnetism

(CA&M Chpt 31)

An electron with intrinsic spin $\frac{1}{2}$ (s = ±1) has intrinsic magnetic moment $\mu = \mu_0 \mathbf{s}$ where $\mu_0 = \frac{e \hbar}{2mc}$ is the Bohr magneton

The interaction energy of the spin with the applied magnetic field is:

$$ \mathcal{E}_H = -\mathbf{\mu} \cdot \mathbf{H} = \mu_0 \mathbf{s} \cdot \mathbf{H} $$
If we take $\hat{H} = H \hat{\sigma}_z$, the above $\delta \mathcal{H}$ then gives the single electron energy eigenvalues:

$$\varepsilon_{ks} = \frac{\hbar^2 k^2}{2m} + s \mu_0 H \quad \text{with} \quad s = \pm 1$$

(parallel) spin up electrons, $s = +1$, increase their energy
(antiparallel) spin down electrons, $s = -1$, decrease their energy

$\Rightarrow$ In equilibrium, this shift of electron energy with $s$ results in a net excess of $s = -1$ electrons

For $H = 0$, the dispersion curves look like

\[ \begin{array}{c}
\text{down} \\
\varepsilon \\
\text{up}
\end{array} \]

$\varepsilon_F$ \quad all states up to $\varepsilon_F$ are filled

$|k|, s = -1$ \quad $|k|, s = +1$

Now imagine turning on a small $H$, but keeping the $s = \pm 1$ populations of electrons the same as when $H = 0$

\[ \begin{array}{c}
\text{down} \\
\varepsilon - \mu_0 H \\
\text{up}
\end{array} \]

$\varepsilon_F + \mu_0 H$ \quad shaded areas are filled electron states

$|k|, s = -1$ \quad $|k|, s = +1$

We see that above cannot remain the ground
state, as the energy will be lowered by
having up electrons at \( \epsilon_F + \mu_0 H, s=+1 \)
convert into down electrons and go into
the empty states at \( \epsilon_F - \mu_0 H, s=-1 \).

The ground state will instead look like

\[
\begin{array}{c}
\text{down} \\
\text{up}
\end{array}
\leftarrow \sim \epsilon_F
\]

and we thus see that there will be more
down than up electrons in the ground state.

Since \( s=\pm 1 \) electrons have magnetic moment
\( \mu = -\mu_0 s \), the system has a net positive
magnetization, magnetized with \( H \).

To see how big \( M \) we need to compute
the number of up electrons that flip into
down electrons when \( H \) is turned on.

We will assume that \( H \) is small enough
that \( \mu_0 H \ll \epsilon_F \). When this is so, we
can ignore the fact that the density of
states has a slight variation with
energy \( \epsilon \) over the range \( \epsilon_F + \mu_0 H \) to \( \epsilon_F - \mu_0 H \)
and assume it to be roughly constant \( g(\epsilon_F) \).
The number of up electrons that flip is then easily computed from the following sketch:

\[
\begin{align*}
&\text{up} \quad \text{down} \\
&\xi = E_F + \mu_{dH} \\
&1/2L, S = -1 \\
&1/2L, S = +1
\end{align*}
\]

The number of up electrons that must flip is therefore

\[
g_+ (E_F) \Delta \xi
\]

where \( g_+ (E_F) = \frac{1}{2} g (E_F) \) is the density of states for up electrons at \( E_F \), which is half the total density of states at \( E_F \), and

\[
\Delta \xi = \frac{1}{2} [\mu_{dH} - (-\mu_{dH})] = \mu_{dH} \text{ is the energy interval that must flip.}
\]

The number of electrons that flip is therefore

\[
\Delta M = \frac{1}{2} g (E_F) \mu_{dH}.
\]

In the new ground state, the number of down electrons is now \( m_0 + \Delta M \), and the number of up electrons is \( m_0 - \Delta M \), where \( m_0 = \frac{1}{2} M \) is the number when \( H = 0 \).
5. The net magnetization is now (at $T=0$)

$$M = \mu_0 \left( m_+ - m_- \right)$$

$$= \mu_0 \left( m_0 + \Delta m - (m_0 - \Delta m) \right)$$

$$= 2\mu_0 \Delta m$$

$$= g(\varepsilon_F) \mu_0^2 H$$

and the Pauli paramagnetic susceptibility is

$$\chi_p = \frac{\partial M}{\partial H} = g(\varepsilon_F) \mu_0^2$$

proportional to the density of states at Fermi energy.

For the free electron gas, we have

$$g(\varepsilon_F) = \frac{3}{2} \frac{n}{\varepsilon_F}$$

\[ \Rightarrow \]

$$\chi_p = \frac{3}{2} \frac{n}{\varepsilon_F} \mu_0^2$$

$$m \sim k_F^3, \quad \varepsilon_F \sim k_F^2, \quad \text{so} \quad \chi_p \sim k_F^2 \sim \frac{1}{(r_s/a_0)}$$

$$\chi_p = \frac{2.59 \times 10^{-6}}{(r_s/a_0)}$$

Corrections to above result at finite $T$ of order

$$\left( \frac{T}{T_F} \right)^2$$

so above is very good at all $T \ll T_F$ and so good at room temperature.
Compare to experiment.

<table>
<thead>
<tr>
<th>Metal</th>
<th>$T_D/ae$</th>
<th>$X_p$ Theory</th>
<th>$X_p$ Ext.</th>
<th>$x10^{-6}$</th>
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<tr>
<td>Li</td>
<td>3.25</td>
<td>0.80</td>
<td>2.0</td>
<td></td>
</tr>
<tr>
<td>Na</td>
<td>3.93</td>
<td>0.66</td>
<td>1.1</td>
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<td>K</td>
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<td>0.8</td>
<td></td>
</tr>
<tr>
<td>Rb</td>
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<td>0.50</td>
<td>0.8</td>
<td></td>
</tr>
<tr>
<td>Cs</td>
<td>5.62</td>
<td>0.46</td>
<td>0.8</td>
<td></td>
</tr>
</tbody>
</table>

It turns out that the discrepancy between theory and experiment is mainly due to having neglected electron-electron interactions.

Note that $X_p$ above is very different from what one gets with classical statistics.

Classically:

$$M \sim \left[ e^{-\mu_0 H/k_B T} + (-1) e^{\mu_0 H/k_B T} \right] (-\mu_0) M$$

$$= \left[ \frac{e^{\mu_0 H/k_B T} - e^{-\mu_0 H/k_B T}}{e^{\mu_0 H/k_B T} + e^{-\mu_0 H/k_B T}} \right] \mu_0 M$$

$$\sim \frac{2 \mu_0 H M}{k_B T} \quad \text{when } \mu_0 H << k_B T$$

$$X_{classical} = \frac{1}{k_B T}$$

So

$$\frac{X_p}{X_{classical}} \sim \left( \frac{T}{T_F} \right) \ll 1$$
Landau Diamagnetism - Landau Levels

Here we wish to consider the effect of the magnetic field on the orbital motion of the conduction electrons. To do so we must solve the quantum mechanical problem of a charged particle moving in a uniform magnetic field.

The geometry we consider is:

\[
\text{uniform } \mathbf{H} = H \mathbf{\hat{z}}
\]

For a particle of charge \( q \) in a static uniform magnetic field, the Hamiltonian is:

\[
\mathcal{H} = \frac{1}{2m} \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right)^2
\]

where \( \mathbf{A} \) is the vector potential, \( \mathbf{H} = \mathbf{\hat{z}} \times \mathbf{A} \)

\( q = -e \) is the charge of the electron.

For \( \mathbf{H} = H \mathbf{\hat{z}} \), we will use \( \mathbf{A} = -\gamma H \mathbf{\hat{x}} \)

Substitute these into \( \mathcal{H} \) to get:
\[ H = \frac{1}{2m} \left( \frac{\hbar^2}{2} \frac{\partial^2}{\partial y^2} - \frac{e}{c} H \frac{\partial}{\partial x} \right)^2 \]

\[ = \frac{1}{2m} \left[ -\frac{\hbar^2}{2} \frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2} \frac{\partial^2}{\partial y^2} + \left( \frac{\hbar^2}{2} \frac{\partial}{\partial x} - \frac{e}{c} H \frac{\partial}{\partial y} \right)^2 \right] \]

We want to find the eigenstates \( \psi \) that solve

\[ H \psi = \varepsilon \psi \]

\( \varepsilon \) is eigenvalue of energy

Any solution of the form

\[ \psi(x,y,z) = e^{ikx} e^{iky} \phi(y) \]

This form is suggested as \( H \) is translationally invariant in \( x \) and \( y \), but not in \( z \) (due to our particular choice for \( \vec{A} \))

Substitute the \( \psi \) into above Schrödinger Equation to get

\[ \frac{1}{2m} \left[ \frac{\hbar^2}{2} \frac{\partial^2}{\partial y^2} + \left( \frac{\hbar k}{c} - \frac{eH}{c} \right)^2 \right] \phi(y) = \varepsilon \phi(y) \]

or

\[ -\frac{\hbar^2}{2m} \frac{\partial^2 \phi}{\partial y^2} + \frac{1}{2m} \left( \frac{\hbar k}{c} - \frac{eH}{c} \right)^2 \phi = (\varepsilon - \frac{\hbar^2 k^2}{2m}) \phi \]

define \( y_0 \) such that \( \frac{\hbar k}{c} \equiv \frac{eH}{c} y_0 \)

\[ -\frac{\hbar^2}{2m} \frac{\partial^2 \phi}{\partial y^2} + \frac{1}{2m} \left( \frac{eH}{c} \right)^2 (y-y_0)^2 \phi = \left( \varepsilon - \frac{\hbar^2 k^2}{2m} \right) \phi \]

define cyclotron frequency \( \omega_c \equiv \frac{eH}{mc} \)

(a classical charged particle in uniform \( \vec{H} \) moves in a circular orbit with angular velocity \( \omega_c \))
Finally we get

\[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{1}{2} m \omega_c^2 (y - y_0)^2 \int \phi(y) = \left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right) \phi(y)\]

This is just the Hamiltonian for a single harmonic oscillator of frequency $\omega_c$ that is centered at $y = y_0$.

We know the eigenvalues of energy of the harmonic oscillator are just

$$\hbar \omega_c (n + \frac{1}{2})$$

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

So we then have

$$\varepsilon - \frac{\hbar^2 k^2}{2m} = \hbar \omega_c (n + \frac{1}{2})$$

or the energy eigenvalues of our particle are

$$\varepsilon = \frac{\hbar^2 k^2}{2m} + \hbar \omega_c (n + \frac{1}{2})$$

or

\[\frac{\hbar^2 k^2}{2m} \quad \frac{\hbar \omega_c (n + \frac{1}{2})}{\hbar \omega_c (n + \frac{1}{2})}

\]

Kinetically energy of

Kinetically energy of

molecule along $\hat{y}$

orbits normal $\hat{y}$

in $xy$ plane $\perp$ to $\hat{z}$

parallel to $\hat{z}$

The wave functions $\phi_n(y)$ are the usual harmonic oscillator wavefunctions (gaussian $\times$ Hermite polynomial) only centered at $y_0$. 


We can therefore write our solution in terms of 3 quantum numbers, \( k_x, k_y, n \):

\[
\psi(k_x, k_y, n) = e^{ikx} e^{iky} \phi_n(y - y_0)
\]

(\( \phi \) is i.o. wavefunction centered at origin)

\[
E(k_x, k_y, n) = \frac{\hbar^2 k_y^2}{2m} + \hbar \omega_c (n + \frac{1}{2})
\]

where \( y_0 = \hbar k_x c / e \hbar = \hbar k_x / m \omega_c \)

Note \( E \) is independent of \( k_x \) so for fixed \( k_y \) and \( n \) there are many degenerate states corresponding to the different possible choices for \( k_x \).

What are the possible values of \( k_x \)?

If we take periodic boundary conditions along \( x \):

\[ \psi(x + 2\pi, y, z) = \psi(x, y, z) \] then we must have:

\[ e^{ikx} = e^{ik(x + 2\pi)} \Rightarrow k_x = \frac{2\pi}{b_x} \text{ (integer)} \]

But \( k_x \) also determines the value of \( y_0 \) about which the wave function is centered in the \( y \)-direction.

Therefore we must have:

\[ 0 \leq y_0 \leq L_y \Rightarrow 0 \leq \hbar k_x \leq \frac{L_y}{m \omega_c} \]

\[ \Rightarrow k_{x \text{ max}} = \frac{L_y m \omega_c}{\hbar} = \frac{L_y e \hbar}{\hbar \frac{m}{mc} \frac{e}{ec}} \]
Combining these two conditions we have the the number of allowed values $k_x$ can take is given by

$$\frac{k_{x \text{ max}}}{\Delta k_x} = \frac{L x L y \frac{eH}{\hbar c}}{\frac{2\pi}{L_x}} = \frac{L x L y \frac{eH}{\hbar c}}{\frac{2\pi}{L_x} \hbar c} = \frac{L x L y H}{\left(\frac{\hbar c}{e}\right)}$$

to get the number of allowed electron states with energy $\frac{\hbar k_x^2 + \hbar c(n + \frac{1}{2})}{2m}$ we should multiply above by a factor of 2 for the two possible spin states.

Degeneracy \( W = 2 \frac{L x L y H}{\left(\frac{\hbar c}{e}\right)} = \frac{\Phi}{\Phi_0} = \frac{\Phi}{\Phi_0} \)

Where \( \Phi = L x L y H \) is the total magnetic flux penetrating the system, and

\( \Phi_0 = \frac{\hbar c}{2e} \) is the unit of magnetic flux and is called the flux quantum.

\( \Phi_0 = 2.07 \times 10^{-7} \) gauss-cm\(^2\)

degeneracy \( n = \frac{\Phi}{\Phi_0} \) = number of flux quanta
Consider now just the motion of the electron in the xy plane. The energy of this motion is

\[ \tilde{E} = E - \frac{\hbar^2 k^2}{2m} = \frac{n + 1/2}{2\mu} \quad n = 0, 1, 2, \ldots \]

The states corresponding to a given value of \( n \) are called the "\( n \)th Landau level". The \( n \)th Landau level has a degeneracy of \( \frac{\pi}{\Phi_0} \), or equivalently, the number of electrons per unit area that one can put into a given Landau level is

\[ \frac{1}{L_x L_y} \frac{\pi}{\Phi_0} = \frac{H}{\Phi_0} \]

We can summarize this by giving the density of states for the energy \( \tilde{E} \) in the xy plane

\[ g_{2D}(\tilde{E}) \, d\tilde{E} = \text{number of electron states per unit area with energy in the range } \tilde{E} \text{ to } \tilde{E} + d\tilde{E} \]

Since there are only states at the discrete energy values \( \frac{n + 1/2}{2\mu} \), \( g_{2D}(\tilde{E}) \) is a sum of \( 8 \)-functions at these discrete values - the amplitude of each \( 8 \)-function is just the degeneracy per area \( H/\Phi_0 \)

\[ g_{2D}(\tilde{E}) = \sum_n \frac{H}{\Phi_0} \delta \left( \tilde{E} - \frac{n + 1/2}{2\mu} \right) \]
We can compare this to the 2D density of states when $H = 0$. From problem (3b) of HW set 1, you will find that at $H = 0$, $g_{2D}(E)$ is a constant.

$$H = 0 : \quad g_{2D}(E) = \frac{m}{\pi \hbar^2}$$

To compare $H = 0$ with $H > 0$, consider

- the average density of state for $H > 0$
- where we average over an energy interval large compared to the spacing between the Landau levels $\hbar \omega_c$.

average density of states

$$\bar{g} = \frac{\text{(2D density spikes in } \Delta E)}{\text{interval width } \Delta E}$$

If we take $\Delta E = M \hbar \omega_c$ for a large integer $M$, then on average there will be $M$ S-function spikes in this interval, so

$$\bar{g} = \frac{M \times \frac{H}{\Phi_0}}{M \hbar \omega_c} = \frac{H}{(\frac{e}{2\pi}) \frac{1}{\hbar (\frac{eH}{mc})}} = \frac{m}{\pi \hbar^2}$$

so average density of state at $H > 0$

$$\bar{g} = \frac{m}{\pi \hbar^2} = \text{constant density of states at } H = 0$$
So turning on the magnetic field branches the energy eigenstates up into discrete levels, but the average number of states per unit energy remains the same (provided we average on interval $\geq \hbar \omega$).