MAGNETISM IN NONINTERACTING ELECTRON GAS

Notes by Luca G Molinari
(Dated: dec. 2016)

In a small magnetic field, even the simple system of non-interacting electrons at small temperature develops complex properties. Magnetization has terms linear in the field (the Pauli paramagnetism and Landau diamagnetism), but complicate terms that oscillate in the inverse field (the de Haas and van Alphen oscillations) also appear. These notes are based on a famous analytic evaluation of such terms by Sondheimer and Wilson.

PACS numbers:

I. INTRODUCTION

In a uniform magnetic field $\vec{H}$, non-interacting classical electrons move along orbits that spiral in the direction of the field with characteristic frequency $\omega_c = eH/mc$. A single orbit is source of a small magnetization with direction opposite to $\vec{H}$ (diamagnetism). The orbits of a cloud of electrons in space give no net current density in bulk, but build a surface current orthogonal to $\vec{H}$. Only the outer electrons feed this diamagnetic field, but since their ratio to the total number vanishes for larger and larger clouds, in thermodynamic limit no magnetization per unit volume results.

If the motion of several electrons is confined in a box, a current also develops along the boundary due to electrons that do not hit the walls. Thus paramagnetic and diamagnetic terms compensate and again, no magnetization survives (van Leeuwen’s theorem, 1921).

The lack of orbital magnetism reflects in classical statistical mechanics in the cancellation of the vector field $\vec{A}$ in the partition function (by a shift of all particles’ momenta $\vec{p}_i$),

$$ Z = \int d^{3N}p \, d^{3N}q e^{-\beta \sum_i \frac{1}{2m}(\vec{p}_i + \vec{A}(\vec{x}_i))^2 + U} $$

thus restoring the partition function of electrons with no magnetic field.

In quantum mechanics orbital magnetism is not suppressed. The energy spectrum is quantized into Landau levels. Landau was the first to compute the $T=0$ diamagnetic levels. The electrons near the walls have higher energies pressed. The energy spectrum is quantized into Landau magnetic field, thus restoring the partition function of electrons with no bulk, but build a surface current orthogonal to $\vec{H}$. Only the outer electrons feed this diamagnetic field, but since their ratio to the total number vanishes for larger and larger clouds, in thermodynamic limit no magnetization per unit volume results.

II. THE BOLTZMANN PARTITION FUNCTION

We consider independent electrons, and allow for an effective mass $m^*$ in the kinetic term and cyclotron frequency, different from the bare mass $m$ that enters in Bohr’s magneton $\mu_B = \hbar/2mc$. Note the relation

$$ \frac{1}{2} \hbar \omega_c = \frac{m^*}{m} \mu_B H $$

The single particle Hamiltonian of an electron in a field $\vec{H} = \text{rot} \vec{A}$ is

$$ h = \frac{1}{2m^*}(\vec{p} + \frac{e}{c} \vec{A})^2 + \mu_B \vec{\sigma} \cdot \vec{H} $$

The energy levels are labelled by the quantum numbers $k = (2\pi/L)r$ $(r \in \mathbb{Z})$, $n = 0,1,2,\ldots$ and $m_s = \pm 1$:

$$ E_{k,n,m_s} = \frac{\hbar^2 k^2}{2m^*} + \hbar \omega_c \left(n + \frac{1}{2}\right) + m_s \mu_B H, $$

The degeneracy of each Landau level is $g = A/(2\pi\ell^2)$ where $A$ is the area transverse to the field, $\ell = (\hbar c/eH)^{1/2}$ is the magnetic length.

The Boltzmann partition function is:

$$ Z_B(\beta, H) = \sum_{k,n,m_s} g e^{-\beta E_{k,n,m_s}} = V \frac{1}{2\pi\ell^2} \left( \frac{m^*}{2\pi\hbar^2\beta} \right)^{1/2} \cosh(\beta \mu_B H) \sinh(\beta \hbar \omega_c/2) $$

It was explained in 1952 by Onsager and Landau and Kosevich as a Fermi surface phenomenon and used since then as a tool to determine the Fermi surface of metals.

The interaction among electrons or the presence of impurities decrease the amplitude of dHvA oscillation, with a reduction factor known as the Dingle factor.

1 More precisely, the induction field $B$ should appear in place of $H$. Both Lorentz force and potential energy of a magnetic dipole depend on the local magnetic field $B = H + 4\pi M$. Since magnetization is an output, dependent also on the particle density, $B$ is unknown. However, for $\chi \ll 1$, we can put $H$ in place of self-consistent field $B$. 

where \( V = AL \) is the volume, \( \beta = 1/(k_B T) \). For low density and high temperature, \( k_B T \gg \mu_B H \), Boltzmann and Fermi statistics yield same results. The magnetization per unit volume is given by Curie’s law:

\[
M = \frac{n}{V} \frac{\partial}{\partial H} \log Z_B = \frac{n \mu_B^2}{k_B T} \left[ 1 - \frac{1}{3} \left( \frac{m}{m^*} \right)^2 \right] H \quad (5)
\]

This is the particle density. We identify a Pauli paramagnetic term (spin) and a Landau diamagnetic term (orbital).

### III. THE GRAN CANONICAL POTENTIAL

For low temperature, Fermi statistics is important and one has to evaluate the gran canonical potential. As shown by Peierls and Rumor, for independent electrons this can be accomplished from the knowledge of the simpler Boltzmann’s partition function, via a Laplace transform:

\[
\Omega = \int_0^\infty dE \, Z(E) \frac{\partial f(E)}{\partial E} \quad (6)
\]

\[
Z(E) = \int_{c-i\infty}^{c+i\infty} \frac{d\beta}{2 \pi i} \frac{e^{\beta E} Z_B(\beta)}{\beta^2} \quad (7)
\]

where \( c > 0 \) and \( f(E) = (1 + e^{\beta(E-\mu)})^{-1} \) is the Fermi occupation number of a state of energy \( E \) and \( \beta \) is a complex variable. A proof is given in the Appendix. For independent electrons in a magnetic field it is

\[
Z(E) = 2V \left( \frac{m^*}{2\pi \hbar^2} \right)^{3/2} \left( \frac{\hbar \omega_c}{2} \right)^{3/2} \left( \frac{2E}{\hbar \omega_c} \right)^{5/2} \quad (8)
\]

The careful evaluation of \( I(x) \) was done by Sondheimer and Wilson. The integrand has a branch cut along the negative-real axis due to \( s^{-7/2} \), and poles \( z = i\pi n, \sigma \neq 0 \). The integral can be evaluated by closing the path and evaluating it by the residue theorem. The same integral can be evaluated by closing the path and evaluating it by the residue theorem. The same integral is the sum of the original integral and an integral on a path along the cut \(-\sigma \) (\( \sigma \) is clock-wise, see Fig. 1). The contribution of the quarter-circles is zero for large radius. Therefore:

\[
I(x) = I_\sigma(x) + I_{\text{poles}}(x)
\]

The term \( I_{\text{poles}} \) will be shown to describe the Pauli and Landau magnetization. The term \( I_{\text{poles}} \) is a series of oscillatory terms in the variable \( x = 2E/\hbar \omega_c \) that will be interpreted as \( d\mathbf{H} \mathbf{A} \) oscillations. As a consequence, \( \Omega_{\text{PL}} + \Omega_{\text{dHVA}} \) will give the partition function as a sum of two terms, \( \Omega_{\text{PL}} + \Omega_{\text{dHVA}} \), as well as the magnetisation

\[
M = -\left[ \frac{\partial \Omega}{\partial H} \right]_{\nu,\mu} = M_{\text{PL}} + M_{\text{dHVA}} \quad (10)
\]

The first two integrals are Hankel’s representation of Gamma function. The magnetic susceptibility is obtained after the dependence on the chemical potential \( \mu \) is replaced by the density, through the equation \( N = -\partial \Omega/\partial \mu \):

\[
\chi = \frac{1}{V} \left[ \frac{\partial M}{\partial H} \right]_{\nu,N} = \chi_{\text{PL}} + \chi_{\text{dHVA}} \quad (11)
\]

Since we are interested in derivatives for small field \( H \), an expansion for large \( s = 2E/\hbar \omega_c \) will be done systematically.

#### A. Pauli and Landau magnetization

The integral along \( \sigma \) is evaluated by exhibiting the singular behaviour in the origin:

\[
z^{-5/2}(\sinh z)^{-1} = z^{-7/2} - \frac{1}{6} z^{-3/2} + R(z)
\]

The remainder \( R \) is just the difference and is finite in \( z = 0 \).

\[
I_\sigma(x) = \frac{1}{2} \int_{\sigma} dz \, e^{z(x+m^*/m) + e^{-z(x-m^*/m)}} \quad (12)
\]

\[
= \frac{1}{2} \left[ \left( x + \frac{m^*}{m} \right)^{\frac{1}{2}} + \left( x - \frac{m^*}{m} \right)^{\frac{1}{2}} \right] \int_{\sigma} dz \, e^{z} z^{-7/2} \]

\[
- \frac{1}{12} \left[ \left( x + \frac{m^*}{m} \right)^{\frac{1}{2}} + \left( x - \frac{m^*}{m} \right)^{\frac{1}{2}} \right] \int_{\sigma} dz \, e^{z^2} z^{-3/2} \]

\[
+ \int_{\sigma} dz \, e^{z^2} \cosh(z \frac{m^*}{m}) R(s) \quad (13)
\]
$x \gg 1$, the binomials are expanded, and the remainder integral is negligible:

$$I_{\sigma}(x) = \frac{8x^{5/2}}{15\sqrt{\pi}} + \frac{x^{1/2}}{\sqrt{\pi}} \left[ \left( \frac{m^*}{m} \right)^2 - \frac{1}{3} \right] + O(x^{-3/2})$$

At $T = 0$ it is $f'(E) = -\delta(\mu - E)$ and the integral $[3]$ is:

$$\Omega_{PL} = -2V \left( \frac{m^*}{2\pi\hbar^2} \right)^{3/2} \left( \frac{\hbar\omega_c}{2} \right)^2 I_{\sigma} \left( \frac{2\mu}{\hbar\omega_c} \right)$$

$$= \Omega_0 - \frac{2}{\sqrt{\pi}} V \mu_B^2 H^2 \mu^{1/2} \left( \frac{m^*}{2\pi\hbar^2} \right)^{3/2} \left[ 1 - \frac{1}{3} \left( \frac{m}{m^*} \right)^2 \right]$$

$\Omega_0$ is the partition function of the Fermi gas in zero field and $T = 0$, eq.$(22)$. The average magnetization at $T = 0$ is

$$M_{PL} = - \left[ \frac{\partial \Omega_{PL}}{\partial H} \right]_{V,\mu}$$

The chemical potential is evaluated as a function of the density, neglecting the rapidly oscillating terms that characterize $\Omega_{dHvA}$:

$$\frac{\mu}{E_F} = 1 + \left( \frac{\mu_B H}{2\mu_0} \right)^2 \left[ 1 - \frac{1}{3} \left( \frac{m}{m^*} \right)^2 \right]$$

where $E_F = \hbar^2(3\pi^2 n)^{2/3}/2m^*$ is the Fermi energy of the ideal gas. Since the correction to $\mu$ is quadratic in $H$, we can replace $\mu$ with $E_F$ in the expression for $M$. A further derivative in $H$, at fixed density, yields the magnetic susceptibility per unit volume:

$$\chi_{PL} = 4 \sqrt{\pi} \mu_B^2 \sqrt{E_F} \left( \frac{m^*}{2\pi\hbar^2} \right)^{3/2} \left[ 1 - \frac{1}{3} \left( \frac{m}{m^*} \right)^2 \right]$$

$$= \mu_B^2 \rho(E_F) \left[ 1 - \frac{1}{3} \left( \frac{m}{m^*} \right)^2 \right]$$

$$\rho(E_F) = \frac{1}{2} n E_F^{-1}$$

$\rho(E_F)$ is the density of states at the Fermi energy of the ideal gas. We recognize a positive (Pauli) paramagnetic term $\chi_P$ and a negative diamagnetic term $\chi_L$ (Landau), which is one third of the former for $m = m^*$.

The Pauli susceptibility only depends on the density $n$, which is usually measured by the parameter $r_s^2$. Indeed it has a very small value:

$$\chi_P = \mu_B^2 \rho(E_F) \left( \frac{1}{r_s^2} \right) \left[ \frac{3}{16\pi} \right] \frac{e^2}{\alpha_0} \frac{\hbar^2}{mc^2}$$

$$= 1.29 \times 10^{-6} \frac{1}{r_s}$$

The above bulk susceptibility was obtained in the thermodynamic limit. Surface corrections would appear for a bounded system, and are always paramagnetic. The present evaluation of $\chi$ is valid in $d = 3$; in $d = 2$ the Boltzmann partition function $Z_B$ does not contain the factor due to longitudinal motion. This causes a pole $z^{-3}$ rather than $z^{-7/2}$ in the integral for $Z(E)$, but the same expression $[16]$ for the Pauli and Landau susceptibilities result.

### B. dHvA oscillations

The contour integral is evaluated by summation of the residues at $z = \pm in\pi$ ($n = 0$ is left out):

$$I_{\text{poles}}(x) = \int_0^\infty dz \cos(z m^*/m) e^{\pi z/2} \sin z$$

$$= - \sum_{n \neq 0} \cos(n \pi m^*/m) e^{\pi z/2} \sin z$$

$$= -\sum_{n=1}^{\infty} \cos(n \pi m^*/m) e^{\pi z/2} \sin z$$

In the evaluation of the integral $[4]$ for $\Omega_{dHvA}$ care must be used in making the limit $T \to 0$, since the function $I_{\text{poles}}(2E/\hbar\omega_c)$ oscillates rapidly on all energy scales. The relevant integral is

$$\int_0^\infty dt \cos(n \pi m^*/m) e^{\pi z/2} \sin z$$

$$= -\sum_{n=1}^{\infty} \cos(n \pi m^*/m) e^{\pi z/2} \sin z$$

$$= -\sum_{n=1}^{\infty} \cos(n \pi m^*/m) e^{\pi z/2} \sin z$$

For $\mu \gg k_B T$, because of the denominator, the lower limit may be replaced by $-\infty$, and the integral is done exactly (GR 3.082.1):

$$= -\frac{1}{2} \int_{-\infty}^{\infty} dt \cos(n \pi m^*/m) e^{\pi z/2} \sin z$$

$$= -\frac{1}{2} \int_{-\infty}^{\infty} dt \cos(n \pi m^*/m) e^{\pi z/2} \sin z$$

Collecting all terms:

$$\Omega_{dHvA} = \frac{V}{2\pi^2} \frac{k_B T \left( e^{H/4\hbar c} \right)^{3/2}}{3/2}$$

$$\times \sum_{n=1}^{\infty} \cos(n \pi m^*/m) \cos(n \pi m^*/m)$$

This term provides the dHvA contribution to the magnetization, which is seen to be a sum of periodic functions
with fundamental frequency

\[ \nu_{d_{\text{HvA}}} = \frac{E_F}{\hbar \omega_c} = \frac{4296.5}{r^2} \left( \frac{1}{H} \right) \text{tesla} \]  

(19)

In \( d = 2 \) neat oscillations were measured in high mobility AlGaAs-GaAs heterostructure at \( T \) around 1K. The experimental curve of M at constant particle density as a function of \( 1/H \) is a sawtooth curve.

IV. APPENDIX

Proof of eq. (6). Consider a system of non-interacting fermions with energy levels \( E_a > 0 \) with degeneracy \( g_a \). The grand canonical potential

\[ \Omega = -\frac{1}{\beta} \sum_a g_a \log(1 + e^{-\beta(E_a - \mu)}) \]

can be evaluated form the Boltzmann partition function \( Z_B(\beta) = \sum_a g_a e^{-\beta E_a} \) via a Laplace transform. Put \( \varphi(E) = -(1/\beta) \log(1 + e^{-\beta(E - \mu)}) \). Its Laplace transform \( \tilde{\varphi}(\beta) = \int_0^\infty dE e^{-\beta E} \varphi(E) \) is well defined for \( \text{Re} \beta > 0 \), with inverse

\[ \varphi(E) = \int_{c-i\infty}^{c+i\infty} \frac{d\beta}{2\pi i} e^{\beta E} \tilde{\varphi}(\beta). \]

The grand canonical potential is:

\[ \Omega = \sum_a g_a \varphi(E_a) = \int_{c-i\infty}^{c+i\infty} \frac{d\beta}{2\pi i} \tilde{\varphi}(\beta) \sum_a g_a e^{\beta E_a} \]

\[ = \int_{c-i\infty}^{c+i\infty} \frac{d\beta}{2\pi i} \tilde{\varphi}(\beta) \frac{Z_B(-\beta)}{\beta^2} \]

The following relation for the resultant of the Laplace transforms is now used (\( x > 0 \)):

\[ \int \frac{ds}{2\pi i} \tilde{f}(s)g(-s)e^{sx} = \int_0^\infty dy f(y) \int \frac{ds}{2\pi i} \tilde{g}(s)e^{s(x-y)} = \int_x^\infty dy f(y)g(y-x) \]

Then: \( \Omega = \int_0^\infty dE \varphi''(E) Z(E) \), where \( Z(E) \) is given in eq. (7).

Example. Boltzmann’s partition function for the ideal electron gas is

\[ Z_B = 2\sum_k e^{-\frac{k^2 a^2}{\pi \hbar^2}} = 2V \left( \frac{m}{2\pi \hbar^2 \beta} \right)^{3/2} \]  

(20)

The auxiliary function is evaluated:

\[ Z(E) = 2V \left( \frac{m}{2\pi \hbar^2} \right)^{3/2} \int_{c-i\infty}^{c+i\infty} \frac{d\beta}{2\pi i} e^{\beta E} \beta^{-7/2} \]

The path is closed as in Fig. [1]. The closed integral is zero being the function analytic inside the contour. Therefore the integral on \( \text{Re} \beta = c \) coincides with the integral on the path of \( \sigma \) shown in Fig. [2]. The latter is Hankel’s representation of the Gamma function:

\[ \frac{1}{\Gamma(z)} = \int_\sigma \frac{ds}{2\pi i} e^{s(z-1)} \]  

(21)

The potential \( \Omega \) is obtained via eq. (6). For \( \beta \mu \gg 1 \) the Fermi distribution is the step function and one gets

\[ \Omega_0 = -\frac{16}{15\sqrt{\pi}} V \left( \frac{m}{2\pi \hbar^2} \right)^{3/2} \mu^{5/2} \]  

(22)

7 J. Jones and March, Theoretical solid state theory, Dover.
8 A. S. Davydov, Teoría del solido, Edizioni Mir, Mosca.
9 L. Onsager, Interpretation of the de Haas-van Alphen effect, Phyl. Mag. 43 (1952) 1006-1008.