

MAGNETISM IN NONINTERACTING ELECTRON GAS

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In a small magnetic field and low temperature, non-interacting electrons develop complex magnetization. Besides linear terms (the *Pauli paramagnetism* and the *Landau diamagnetism*), magnetization shows complicate oscillations as function in the inverse field (the *de Haas and van Alphen oscillations*). These notes are based on a famous analytic evaluation of such terms by Sondheimer and Wilson.

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I. INTRODUCTION

In a uniform magnetic field $\mathbf{H}$, 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 the field (diamagnetism). The orbits of a cloud of electrons in space give no net current density in bulk, but build a surface current density orthogonal to $\mathbf{H}$. Only the outer electrons feed this diamagnetic field, and since their number ratio to the total 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 bounce on it. This current density is opposite and exactly cancels the surface current 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 $\mathbf{A}$ in the partition function by a shift of all $\mathbf{p}_j$ in

$$Z = \int \prod_j d\mathbf{p}_j d\mathbf{x}_j e^{-\beta \sum_i \frac{1}{2m} (\mathbf{p}_i + \frac{e}{c} \mathbf{A}(\mathbf{x}_i))^2 + U(\mathbf{x}_1 \dots \mathbf{x}_N)}$$

that restores the partition function of free electrons.

In quantum mechanics orbital magnetism is not suppressed. The energy spectrum is quantized into Landau levels that, in open space, are the levels of displaced harmonic oscillators. Landau was the first to compute the $T=0$ diamagnetic susceptibility χ_L (1930), and found a value equal to $-1/3$ of the (paramagnetic) susceptibility χ_P due to spin found by Pauli.

Landau also noticed, for small T , that there are further nonlinear terms that contribute to magnetization of free electrons, with a complex structure.

In 1930 de Haas and van Alphen discovered that the magnetic susceptibility of Bismuth is not constant at low temperature, but oscillates as a function of $1/H$. The effect was then found in many other metals, in the range

$$E_F \gg \hbar\omega_c \gg k_B T$$

In the early experiment by Schoenberg² in Kapitza's institute, a light pure Bismuth crystal was suspended to

a long thin quartz wire carrying a mirror, refrigerated in Helium gas. The mechanical couple due to magnetization in a magnetic field of 9.5 kgauss was measured by light deflection. The theory for anisotropic system was put forward by Blackman¹. Onsager¹³ (1952) and Lifshitz and Kosevich¹¹ explained the oscillations as a Fermi surface phenomenon, and their measure is used since then as a tool to determine the Fermi surface^{10,12}.

The interaction among electrons or the presence of impurities decrease the amplitude of dHvA oscillation, with a reduction factor known as the *Dingle factor*⁶.

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 $\mu_B = e\hbar/2mc$. Note the relation

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

The single particle Hamiltonian of an electron in a field $\mathbf{H} = \text{rot}\mathbf{A}$ is¹

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

For a uniform field along the z axis, in the Landau gauge $\mathbf{A} = (0, xH, 0)$ the Hamiltonian is separable. The energy levels are labelled by the quantum numbers $k = (2\pi/L)r$ ($r \in \mathbb{Z}$), $n = 0, 1, 2, \dots$ and $m_s = \pm 1$:

$$E_{k,n,m_s} = \frac{\hbar^2 k^2}{2m^*} + \hbar\omega_c \left(n + \frac{1}{2}\right) + m_s \mu_B H, \quad (3)$$

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

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 .

The Boltzmann partition function is:

$$\begin{aligned} Z_B(\beta, H) &= \sum_{k, n, m_s} g e^{-\beta E_{k, n, m_s}} \\ &= \frac{V}{2\pi\ell^2} \sqrt{\frac{m^*}{2\pi\hbar^2\beta}} \frac{\cosh(\beta\mu_B H)}{\sinh(\beta\hbar\omega_c/2)} \end{aligned} \quad (4)$$

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 magnetisation per unit volume is given by Curie's law:

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

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

III. THE GRAN CANONICAL POTENTIAL

At low temperature Fermi statistics is important, and it is necessary to evaluate the gran canonical potential. As shown by Peierls and Rumor, for non-interacting electrons this can be accomplished from the knowledge of the simpler Boltzmann's partition function, via a Laplace transform:

$$\Omega = \int_0^\infty dE \zeta(E) \frac{\partial f(E)}{\partial E} \quad (6)$$

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

where $c > 0$ and $f(E) = (e^{\beta(E-\mu)} + 1)^{-1}$ is the Fermi occupation number of a state of energy E and β has become a complex variable (see Appendix).

For the electrons gas in a magnetic field it is

$$\zeta(E) = 2V \left(\frac{m^*}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left(\frac{\hbar\omega_c}{2} \right)^{\frac{5}{2}} \text{I} \left(\frac{2E}{\hbar\omega_c} \right) \quad (8)$$

$$\text{I}(x) = \int_{c-i\infty}^{c+i\infty} \frac{dz}{2\pi i} \frac{\cosh(z m^*/m)}{z^{5/2} \sinh z} e^{zx} \quad (9)$$

The careful evaluation of $\text{I}(x)$ was done by Sondheimer and Wilson³ (see also⁴ for the same analysis, or⁵ for an approach based on polylog functions).

The integrand has a branch cut along the negative-real axis due to $z^{-7/2}$, and poles $z = in\pi$, $n \neq 0$. The integral can be evaluated by the residue theorem. The contour path is shown in Fig.1. The contribution of the quarter-circles is zero for large radius. Therefore:

$$\text{I}(x) = \text{I}_{\text{cut}}(x) + \text{I}_{\text{poles}}(x)$$

The term I_{cut} will describe the Pauli and Landau magnetization. The term I_{poles} is a series of oscillatory terms in the variable $x = 2E/\hbar\omega_c$ that gives dHvA oscillations.

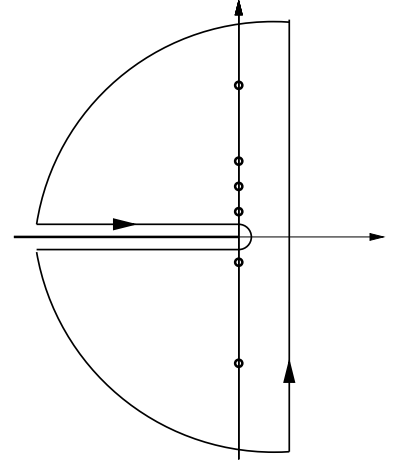


FIG. 1: The path $(c - i\infty, c + i\infty)$ in the complex s -plane is completed into the oriented contour C that avoids the cut $\text{Re } s < 0$ and encloses simple poles on the imaginary axis. While the two arcs do not contribute to the integral, the integral on the path $(-\infty + i\epsilon, \infty - i\epsilon)$ enclosing the cut does, and is subtracted (added with orientation reversed: this is path σ).

As a consequence, eq.(6) gives the partition function as the sum of two terms, $\Omega_{\text{PL}} + \Omega_{\text{dHvA}}$.

The magnetisation is

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

The magnetic susceptibility is obtained after replacing the chemical potential μ by the density, through the equation $N = -\partial\Omega/\partial\mu$:

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

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

A. Pauli and Landau magnetization

The integral along σ is evaluated by exhibiting the singular behaviour at the origin:

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

The remainder R is finite at $z = 0$.

$$\text{I}_{\text{cut}}(x) = \frac{1}{2} \int_{\sigma} \frac{dz}{2\pi i} \frac{e^{z(x+m^*/m)} + e^{z(x-m^*/m)}}{z^{5/2} \sinh z} \quad (12)$$

$$\begin{aligned} &= \frac{1}{2} \left[\left(x + \frac{m^*}{m} \right)^{\frac{5}{2}} + \left(x - \frac{m^*}{m} \right)^{\frac{5}{2}} \right] \int_{\sigma} \frac{dz}{2\pi i} e^z z^{-7/2} \\ &\quad - \frac{1}{12} \left[\left(x + \frac{m^*}{m} \right)^{\frac{1}{2}} + \left(x - \frac{m^*}{m} \right)^{\frac{1}{2}} \right] \int_{\sigma} \frac{dz}{2\pi i} e^z z^{-3/2} \\ &\quad + \int_{\sigma} \frac{dz}{2\pi i} \cosh\left(z \frac{m^*}{m}\right) R(z) e^{zx} \end{aligned} \quad (13)$$

The first two integrals are Hankel's representation of the Gamma function, (27). Since the field H is weak, i.e. $x \gg 1$, the binomials are expanded, while the remainder integral is negligible:

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

At $T = 0$ it is $f'(E) = -\delta(\mu - E)$ and the integral (6) is:

$$\begin{aligned} \Omega_{\text{PL}} &= -2V \left(\frac{m^*}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left(\frac{\hbar\omega_c}{2} \right)^{\frac{5}{2}} I_{\text{cut}} \left(\frac{2\mu}{\hbar\omega_c} \right) \\ &= \Omega_0 - \frac{2V}{\sqrt{\pi}} \mu_B^2 H^2 \mu^{1/2} \left(\frac{m^*}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] \end{aligned} \quad (14)$$

Ω_0 is the partition function of the Fermi gas in zero field and $T = 0$, eq.(28). The average magnetization at $T = 0$ is

$$M_{\text{PL}} = - \left[\frac{\partial \Omega_{\text{PL}}}{\partial H} \right]_{V, \mu} \quad (15)$$

The chemical potential is evaluated as a function of the density, neglecting the rapidly oscillating terms that characterize Ω_{dHvA} . Inversion of $N = -\partial \Omega_{\text{PL}} / \partial \mu$ gives:

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

where $E_F = \hbar^2(3\pi^2 n)^{2/3}/2m^*$ is the Fermi energy of the ideal gas. Since the correction to μ is quadratic in H , we can replace μ with E_F in the expression for M :

$$\frac{M_{\text{PL}}}{V} = \frac{4H}{\sqrt{\pi}} \mu_B^2 \sqrt{E_F} \left(\frac{m^*}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] \quad (16)$$

A further derivative in H , at fixed density, yields the magnetic susceptibility per unit volume:

$$\begin{aligned} \chi_{\text{PL}} &= \frac{4}{\sqrt{\pi}} \mu_B^2 \sqrt{E_F} \left(\frac{m^*}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] \\ &= \mu_B^2 \rho(E_F) \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] \end{aligned} \quad (17)$$

$\rho(E_F) = \frac{3}{2} n E_F^{-1}$ is the density of states at the Fermi energy of the ideal gas. We recognize a positive (Pauli) paramagnetic term χ_{P} and a negative diamagnetic term χ_{L} (Landau), which is one third of the former when $m = m^*$.

The Pauli susceptibility only depends on the density n , which can be measured by the parameter r_s^2 . It has a very small value:

$$\chi_{\text{P}} = \mu_B^2 \rho(E_F) = 1.29 \times 10^{-6} \frac{1}{r_s} \quad (18)$$

² The parameter r_s measures the average radius of the empty sphere available per particle in units of Bohr's radius a_0 : $\frac{4}{3}\pi(a_0 r_s)^3 = \frac{1}{n}$. For metals it is $r_s \approx 3 - 6$.

The above bulk susceptibility was obtained in the thermodynamic limit. Surface corrections would appear in a bounded system, and are always paramagnetic⁷.

The present evaluation of χ 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 $\zeta(E)$, but the same expression (17) for the Pauli and Landau susceptibilities result.

B. dHvA oscillations

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

$$\begin{aligned} I_{\text{poles}}(x) &= \int_C \frac{dz}{2\pi i} \frac{\cosh(z m^*/m)}{z^{5/2} \sinh z} e^{zx} \\ &= - \sum_{n \neq 0} \frac{\cos(n\pi m^*/m)}{(n\pi)^{5/2}} e^{i\pi(n x - \frac{1}{4} \text{sign } n)} \\ &= -2 \sum_{n=1}^{\infty} \frac{\cos(n\pi m^*/m)}{(n\pi)^{5/2}} \cos(n\pi x - \frac{\pi}{4}) \end{aligned}$$

In evaluating the integral (6) for Ω_{dHvA} care must be used for the limit $T \rightarrow 0$, since the function $I_{\text{poles}}(2E/\hbar\omega_c)$ oscillates rapidly at all energy scales. The relevant integral is

$$\begin{aligned} &\int_0^{\infty} dE \cos \left(n\pi \frac{2E}{\hbar\omega_c} - \frac{\pi}{4} \right) f'(E) \\ &= -\frac{\beta}{4} \int_0^{\infty} dE \frac{\cos(n\pi \frac{2E}{\hbar\omega_c} - \frac{\pi}{4})}{\cosh^2(\frac{1}{2}\beta(E - \mu))} \\ &= -\frac{1}{2} \int_{-\frac{1}{2}\beta\mu}^{\infty} dt \frac{\cos(\frac{4n\pi}{\beta\hbar\omega_c} t + 2n\pi \frac{\mu}{\hbar\omega_c} - \frac{\pi}{4})}{\cosh^2 t} \end{aligned}$$

For $\mu \gg k_B T$, because of the denominator, the lower limit may be replaced by $-\infty$, and the integral is done exactly¹⁵:

$$\begin{aligned} &= -\frac{1}{2} \cos \left(n\pi \frac{2\mu}{\hbar\omega_c} - \frac{\pi}{4} \right) \int_{-\infty}^{\infty} dt \frac{\cos(\frac{4n\pi}{\beta\hbar\omega_c} t)}{\cosh^2 t} \\ &= -\frac{2n\pi^2 \cos(n\pi \frac{2\mu}{\hbar\omega_c} - \frac{\pi}{4})}{\beta\hbar\omega_c \sinh(n\pi \frac{2\pi^2}{\beta\hbar\omega_c})} \end{aligned} \quad (19)$$

Collecting all terms:

$$\begin{aligned} \Omega_{\text{dHvA}} &= \frac{V}{2\pi^2} k_B T \left(\frac{eH}{4\hbar c} \right)^{3/2} \times \\ &\times \sum_{n=1}^{\infty} \frac{\cos(n\pi m^*/m)}{n^{3/2}} \frac{\cos(n\pi \frac{2\mu}{\hbar\omega_c} - \frac{\pi}{4})}{\sinh(n\pi \frac{2\pi^2}{\beta\hbar\omega_c})} \end{aligned}$$

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

with fundamental frequency

$$\nu_{\text{dHvA}} = \frac{E_F}{\hbar\omega_c} = \frac{4296.5}{r_s^2} \left(\frac{1}{H} \right)_{\text{tesla}} \quad (20)$$

In $d = 2$ neat oscillations were measured in high mobility AlGaAs-GaAs heterostructure⁹ at T around 1K. The experimental curve of M at constant particle density as a function of $1/H$ is a sawtooth curve.

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 and the Boltzmann partition function are:

$$\Omega(\beta) = -\frac{1}{\beta} \sum_a g_a \log(1 + e^{-\beta(E_a - \mu)}) \quad (21)$$

$$Z_B(\beta) = \sum_a g_a e^{-\beta E_a} \quad (22)$$

If $\rho(E) = dN/dE$ is the level density they become, after an integration by parts:

$$\begin{aligned} \Omega(\beta) &= - \int_0^\infty dE N(E) f(E) \\ Z_B(\beta) &= \beta \int_0^\infty dE N(E) e^{-\beta E} \end{aligned}$$

Therefore, $Z_B(\beta)/\beta$ is the Laplace transform of $N(E)$, that counts the states with energy below E . It is convenient to go further, and assume that $N(E) = d\zeta(E)/dE$. After another integration by parts:

$$\Omega(\beta) = \int_0^\infty dE \zeta(E) f'(E) \quad (23)$$

$$Z_B(\beta) = \beta^2 \int_0^\infty dE \zeta(E) e^{-\beta E} \quad (24)$$

The function $\zeta(E)$ is obtained by Laplace-inversion of the integral (24):

$$\zeta(E) = \int_{c-i\infty}^{c+i\infty} \frac{d\beta}{2\pi i} \frac{Z_B(\beta)}{\beta^2} e^{\beta E} \quad (25)$$

The evaluation of this integral gives Ω , eq.(23).

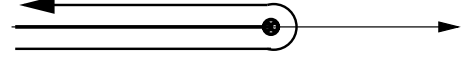


FIG. 2: The path σ around the cut.

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

$$Z_B(\beta) = 2 \sum_{\mathbf{k}} e^{-\frac{\hbar^2 \mathbf{k}^2}{2m}} = 2V \left(\frac{m}{2\pi\hbar^2\beta} \right)^{3/2} \quad (26)$$

The auxiliary function is evaluated:

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

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 σ shown in Fig. (2). The latter is Hankel's representation of the Gamma function:

$$\frac{1}{\Gamma(z)} = \int_{\sigma} \frac{ds}{2\pi i} e^s s^{-z} \quad (27)$$

The potential Ω at $T = 0$ is

$$\Omega_0 = V \frac{16}{15\sqrt{\pi}} \left(\frac{m}{2\pi\hbar^2} \right)^{3/2} \mu^{5/2} \quad (28)$$

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