MAGNETISM IN NONINTERACTING ELECTRON GAS

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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.

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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 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 $\vec{A}$ in the partition function (by a shift of all particles' momenta $\vec{p}_i$),

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

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. The electrons near the walls have higher energies than electrons in bulk, and hence a different statistical weight. This causes a net orbital diamagnetism to arise. Landau was the first to compute the T=0 diamagnetic susceptivity χ_L (1930), and found a value equal to $-1/3$ of Pauli's (paramagnetic) susceptivity χ_P due to spin. 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 Schoenberg[3] in Kapitza's institute, a pure light Bysmuth 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 Blackman[2]. Onsager[12] (1952) and Lifshitz and Kosevich[10] explained the oscillations as a Fermi surface phenomenon, and their measure is used since then as a tool to determine the Fermi surface[9,11]. The interaction among electrons or the presence of impurities decrease the amplitude of dHvA oscillation, with a reduction factor known as the *Dingle factor*[4].

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

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

The single particle Hamiltonian of an electron in a field $\vec{H} = \mathrm{rot}\vec{A}$ is[1]

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

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

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

The degeneracy of each Landau level is $g = A/(2\pi\ell^2)$ where A is the area transverse to the field, $\ell =$

[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.

$(\hbar c/eH)^{1/2}$ is the magnetic length.
The Boltzmann partition function is:

$$Z_B(\beta,H) = \sum_{k,n,m_s} g\, e^{-\beta E_{k,n,m_s}} = V\frac{1}{2\pi\ell^2}\left(\frac{m^*}{2\pi\hbar^2\beta}\right)^{1/2}\frac{\cosh(\beta\mu_B H)}{\sinh(\beta\hbar\omega_c/2)} \quad (4)$$

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 magnetization 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

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:

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

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

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

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

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

The careful evaluation of $\mathrm{I}(x)$ was done by Sondheimer and Wilson[1] (see also[14] for the same analysis, or[6] for an approach based on polylog functions). The integrand has a branch cut along the negative-real axis due to $s^{-7/2}$, and poles $z = in\pi$, $n \neq 0$. The integral can be evaluated by the residue theorem. The contour integral with path shown in Fig.1 is the sum of the original one and the integral along a path $-\sigma$ surrounding the cut (then σ is clock-wise). The contribution of the quarter-circles is zero for large radius. Therefore:

$$\mathrm{I}(x) = \mathrm{I}_\sigma(x) + \mathrm{I}_{\mathrm{poles}}(x)$$

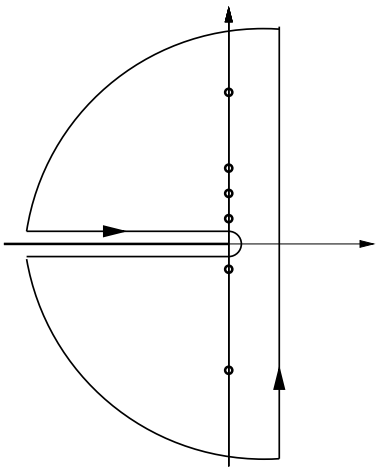

FIG. 1: The path $(c - i\infty, c + i\infty)$ in the complex s-plane is completed into the oriented contour C that avoids the cut Re $s < 0$ and encloses simple poles on the imaginary axis. While the two arcs do not contribute to the integral, the integral on the path $(-\infty + i\epsilon, \infty -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

The term I_σ will be shown to describe the Pauli and Landau magnetization. The term $\mathrm{I}_{\mathrm{poles}}$ is a series of oscillatory terms in the variable $x = 2E/\hbar\omega_c$ that will be interpreted as dHvA oscillations.
As a consequence, (6) will give the partition function as a sum of two terms, $\Omega_{\mathrm{PL}} + \Omega_{\mathrm{dHvA}}$. The magnetisation is

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

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

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

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

A. Pauli and Landau magnetization

The integral along σ 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 $z = 0$.

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

$$= \frac{1}{2}\left[\left(x+\frac{m^*}{m}\right)^{\frac{5}{2}} + \left(x-\frac{m^*}{m}\right)^{\frac{5}{2}}\right]\int_\sigma \frac{dz}{2\pi i}e^z z^{-7/2}$$

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

$$+ \int_\sigma \frac{dz}{2\pi i}e^{zx}\cosh(z\frac{m^*}{m})R(s) \tag{13}$$

The first two integrals are Hankel's representation of Gamma function, (21). Since the field H is weak, i.e. $x \gg 1$, the binomials are expanded, and the remainder integral is negligible:

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

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

$$\Omega_{\mathrm{PL}} = -2V\left(\frac{m^*}{2\pi\hbar^2}\right)^{3/2}\left(\frac{\hbar\omega_c}{2}\right)^{5/2}\mathrm{I}_\sigma\left(\frac{2\mu}{\hbar\omega_c}\right) \tag{14}$$

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

Ω_0 is the partition function of the Fermi gas in zero field and $T = 0$, eq.(22). The average magnetization at $T = 0$ is

$$M_{\mathrm{PL}} = -\left[\frac{\partial\Omega_{PL}}{\partial H}\right]_{V,\mu} \tag{15}$$

The chemical potential is evaluated as a function of the density, neglecting the rapidly oscillating terms that characterize Ω_{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 μ is quadratic in H, we can replace μ with E_F in the expression for M. A further derivative in H, at fixed density, yields the magnetic susceptibility per unit volume:

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

$$= \mu_B^2\,\rho(E_F)\left[1 - \frac{1}{3}\left(\frac{m}{m^*}\right)^2\right] \tag{16}$$

$\rho(E_F) = \frac{3}{2}nE_F^{-1}$ 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 for $m = m^*$.

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

$$\chi_{\mathrm{P}} = \mu_B^2\rho(E_F) = \frac{1}{\pi r_s}\left(\frac{3}{16\pi}\right)^{2/3}\frac{e^2/a_0}{mc^2}$$

$$= 1.29\times 10^{-6}\frac{1}{r_s} \tag{17}$$

The above bulk susceptibility was obtained in the thermodynamic limit. Surface corrections would appear for a bounded system, and are always paramagnetic[5]. 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 (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):

$$\mathrm{I}_{\mathrm{poles}}(x) = \int_C \frac{dz}{2\pi i}e^{zx}\frac{\cosh(z\,m^*/m)}{z^{5/2}\sinh z}$$

$$= -\sum_{n\neq 0}\frac{\cos(n\pi m^*/m)}{(n\pi)^{5/2}}e^{i\pi(nx - \frac{1}{4}\mathrm{sign}\,n)}$$

$$= -2\sum_{n=1}^{\infty}\frac{\cos(n\pi m^*/m)}{(n\pi)^{5/2}}\cos(n\pi x - \frac{\pi}{4})$$

In the evaluation of the integral (6) for Ω_{dHvA} care must be used in making the limit $T \to 0$, since the function $\mathrm{I}_{\mathrm{poles}}(2E/\hbar\omega_c)$ oscillates rapidly at all energy scales. The relevant integral is

$$\int_0^\infty dE\cos\left(n\pi\frac{2E}{\hbar\omega_c} - \frac{\pi}{4}\right)f'(E)$$

$$= -\frac{\beta}{4}\int_0^\infty dE\frac{\cos(n\pi\frac{2E}{\hbar\omega_c} - \frac{\pi}{4})}{\cosh^2(\frac{1}{2}\beta(E-\mu))}$$

$$= -\frac{1}{2}\int_{-\frac{1}{2}\beta\mu}^\infty dt\frac{\cos(\frac{4n\pi}{\beta\hbar\omega_c}t + 2n\pi\frac{\mu}{\hbar\omega_c} - \frac{\pi}{4})}{\cosh^2 t}$$

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

[2] The parameter r_s measures the average radius of the empty sphere available per particle in units of Bohr's radius a_0: $\frac{4}{3}\pi(a_0r_s)^3 = \frac{1}{n}$. For metals it is $r_s \approx 3 - 6$.

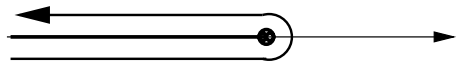

FIG. 2: The path σ around the cut.

exactly (GR 3.982.1):

$$= -\frac{1}{2}\cos\left(n\frac{2\pi\mu}{\hbar\omega_c} - \frac{\pi}{4}\right)\int_{-\infty}^{\infty} dt \frac{\cos(\frac{4n\pi}{\beta\hbar\omega_c}t)}{\cosh^2 t}$$
$$= -\frac{2n\pi^2}{\beta\hbar\omega_c}\frac{\cos(n\frac{2\pi\mu}{\hbar\omega_c} - \frac{\pi}{4})}{\sinh(n\frac{2\pi^2}{\beta\hbar\omega_c})} \qquad (18)$$

Collecting all terms:

$$\Omega_{\rm dHvA} = \frac{V}{2\pi^2}k_BT\left(\frac{eH}{4\hbar c}\right)^{3/2} \times$$
$$\times \sum_{n=1}^{\infty}\frac{\cos(n\pi m^*/m)}{n^{3/2}}\frac{\cos(n\frac{2\pi\mu}{\hbar\omega_c} - \frac{\pi}{4})}{\sinh(n\frac{2\pi^2}{\beta\hbar\omega_c})}$$

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

$$\nu_{\rm dHvA} = \frac{E_F}{\hbar\omega_c} = \frac{4296.5}{r_s^2}\left(\frac{1}{H}\right)_{\rm tesla} \qquad (19)$$

In $d = 2$ neat oscillations were measured in high mobility AlGaAs-GaAs heterostructure[8] 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 gran canonical potential

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

can be evaluated from the Boltzmann partition function

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

Put $\varphi(E) = -(1/\beta)\log(1 + e^{-\beta(E-\mu)})$. Its Laplace transform $\tilde\varphi(s) = \int_0^\infty dE e^{-sE}\varphi(E)$ is well defined for $\mathrm{Re}\, s > -\beta$, with inverse

$$\varphi(E) = \int_{c-i\infty}^{c+i\infty}\frac{ds}{2\pi i}e^{sE}\tilde\varphi(s).$$

The grand canonical potential is:

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

The formula for the *resultant*[13] is now used with $x = 0$:

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

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

$$Z_B(\beta) = 2\sum_{\mathbf{k}} e^{-\frac{\hbar^2k^2}{2m}} = 2V\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2} \qquad (20)$$

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 $\mathrm{Re}\ \beta = c$ coincides with the integral on the path σ shown in Fig. (2). The latter is Hankel's representation of the Gamma function:

$$\frac{1}{\Gamma(z)} = \int_\sigma\frac{ds}{2\pi i}e^s s^{-z} \qquad (21)$$

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

$$\Omega_0 = -\frac{16}{15\sqrt{\pi}}V\left(\frac{m}{2\pi\hbar^2}\right)^{3/2}\mu^{5/2} \qquad (22)$$

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