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Corso di laurea triennale in Fisica



Diamagnetism and de Haas-van Alphen oscillations in the electronic gas

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PACS: 05.30.d

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Anno Accademico 2008 - 2009

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February 13, 2010

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Abstract

We consider a Fermi gas in a magnetic field \vec{H} . We compute analytically the grand canonical potential Ω and derive the magnetic susceptibility χ . Ω can be evaluated with the method of Peierls, via a Laplace inverse transform of the Boltzmann canonical partition function $Z(\beta)$. The integral in the complex plane is evaluated over an appropriate contour, applying the theorem of residues. The calculation is done for $D=3$ and $D=2$. At low temperature, an oscillatory behaviour of Ω arises, which is the experimentally observed de Haas-van Alphen (dHvA) effect for metals.

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1 Introduction

The de Haas-van Alphen effect (dHvA) is a non-linear, oscillatory behaviour of magnetization in metals, as the external magnetic field \vec{H} is changed. These oscillations are found in other physical quantities of metals, as magnetoresistivity (Shubnikov-de Haas effect), specific heat, sound attenuation; they are caused by the quantization of the energy levels of electrons (the *Landau Levels*) in a magnetic field.

Magnetization M in statistical mechanics is the variable

$$M := -\frac{\partial \mathcal{E}}{\partial H}$$

where \mathcal{E} is the thermodynamical potential in the chosen description (it can be the internal energy, Helmholtz free energy, Gibbs energy, the grand canonical potential Ω , etc.).

A quantum mechanical treatment of free electrons gives three terms for the magnetic susceptibility χ :

$$\chi := \frac{1}{V} \frac{\partial M}{\partial H} = \chi_P + \chi_L + \chi_{osc}$$

The first term is due to the spin-field interaction (Pauli's paramagnetic χ_P); the second term, Landau's diamagnetic χ_L , accounts for the orbital motion of the charged electron in the magnetic field which, like a microscopic loop of current, generates a magnetic moment; the last term is not constant like the other two, but is an oscillating function of $1/H$ - plotted against H , it gives a sawtooth curve.

This last term is the dHvA effect, and is detectable in the regime $\mu_B H \gg k_b T$, high magnetic fields and low temperatures, as we shall see. These three terms - and all magnetism, indeed, as shown by Bohr and van Leeuwen - can be explained only with a quantum mechanical description.

The dHvA effect is one of the most powerful tool for measuring the Fermi surface (FS) of metals, which determines most of the relevant electronic properties. The FS is mapped out by its cross sectional extremal areas A_{extr} , measured for different directions, since A_{extr} is proportional to the frequency of the dHvA oscillations. In fact, all properties that depend on the density of states show an oscillatory dependence on $1/H$.

1.1 Outlook of this work

Here we outline the structure of this article.

A general introduction is given, with a short summary of the historical development of the theory and the experimental advancements related to the de Haas-van Alphen (dHvA) effect (§1.2).

We are interested in deriving magnetic quantities, as susceptibility, from theoretical considerations. This theory will be done after a presentation of the single-particle Hamiltonian that governs the energy of free, noninteracting electrons in an external magnetic field, uniform in space (§2).

Such a system shows a typical quantum mechanical behaviour, with discrete energies called *Landau levels* (§2.1). We make some qualitative considerations over the eigenfunctions of the energy, which show consistent differences for far and near the edges of the sample, determining respectively bulk and edge states. we will consider the *degeneracy* of the energy levels, and show the connection to the Fermi surface of metals.

In section (§3) we apply statistical mechanics (SM) to investigate the properties of the gas of electrons. In doing that, we see how the quantum mechanics of single electrons affect the macroscopic ensemble.

Through SM it is possible to trace the mechanical meaning of thermodynamical quantities, such as magnetization M and susceptibility χ . Classical SM is governed by Boltzmann probability and for high temperatures it describes quantum systems too (§3.1). For low temperatures though, it is necessary to apply Fermi-Dirac statistics, since Pauli's exclusion principle plays an important role in the distribution of the particles density. Moreover, quantum statistical systems are appropriately described through the grand canonical ensemble (§3.2), in which the number of particles N of the system may vary.

Hence, we use Peierls' method to switch from a canonical to a grand canonical description of the system, in a rigorous mathematical way (§3.3). We summarize the calculation (§4) done by Sondheimer and Wilson for the system in 3D. It takes advantage of well-known tools of complex analysis, as the theorem of residues to evaluating a Laplace inverse transform.

At last, we put forth the calculation for a 2D system (§5), which is - to our knowledge - the original feature of this work.

The calculations show that both in 3D and 2D, magnetization is the sum of three terms: diamagnetic, paramagnetic, and dHvA contributions. While

the diamagnetic and paramagnetic susceptibilities are independent from the external field, and are the leading terms for high temperatures, the dHvA susceptibility shows an oscillatory dependence on the inverse field $1/H$, and is not negligible in the small temperatures-strong magnetic field regime.

In the appendix (§A) there is a basic description of the mathematical tools we use, namely the Laplace transform (§A.1), Peierls' method (A.2), the calculus of residues (§A.3) and Hankel's representation of the Gamma function (§A.4).

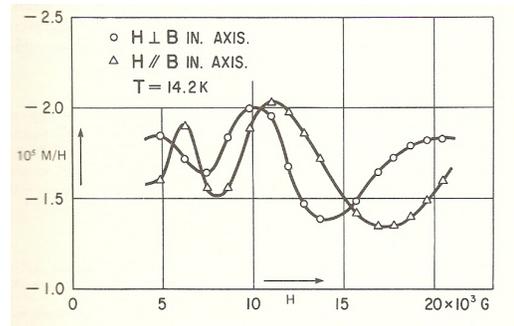


Figure 1: First observation of oscillatory dependence of susceptibility (vertical axis) on the magnetic field strength (horizontal axis) in a pure crystal of bismuth. (de Haas, van Alphen, 1930) [1].

1.2 Historical overview

Bohr (1911) and then Van Leeuwen (1919) pointed out how no magnetic effect can arise from a classical mechanical system at thermal equilibrium. In the 1930s, Landau explained the mechanism underlying *diamagnetism*; the electronic orbit generates a magnetic moment that couples with the magnetic field, diminishing it. This magnetization is opposite to Pauli *paramagnetism*, which explains the tendency of the electron spin to align to the field, increasing it. The two effects are in contrast, and the deriving magnetic susceptibilities, for free electrons are $\chi_L = -\frac{1}{3}\chi_P$.

At low temperatures and in high magnetic fields, experiments showed how susceptibility was not independent from the magnetic field. Until then, a straight line was expected, whose slope represents the metal's susceptibility - a constant that indicates its response in magnetization as the field is

increased. Instead, a sawtooth curve was plotted. Such oscillating behaviour of magnetization is the de Haas-van Alphen effect (dHvA), discovered in December 1930 in crystal bismuth, as visible in Fig. (1).

Earlier that year, Landau had independently made a theoretical prediction of such phenomenon, deriving it from the quantum mechanics that governs the electron. A free electron in a uniform magnetic field moves in a spiral that points in the direction of the field. That is, seen in the direction of the field, the electron orbit is a circle, whose radius depends on the strength of the field. The difference between classical and quantum theory is that in the latter (in a semi-classical picture), the radius r_c can take discrete values only. Such orbits correspond to discrete energy levels, the Landau Levels (LL).

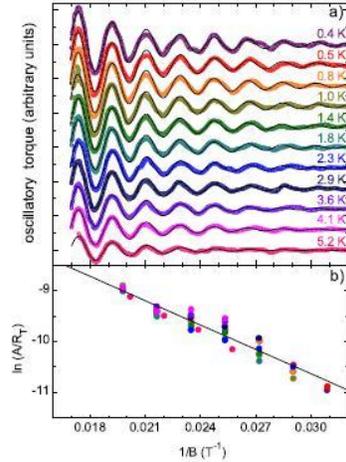


Figure 2: (a) Field dependence of the oscillatory part of the torque for the various temperatures explored and (b) corresponding Dingle plots. From Jaudet, (2008) [2].

Magnetization and other thermodynamical quantities (such as temperature) can be explained as the macroscopic outcome of a microscopic interaction that is averaged on many particles, for a given probability (which, in turn, defines a *statistics*). Mechanical statistics is indeed the branch of physics that tries to account for this connection.

Landau made a complete analytical derivation of the free energy by using the Poisson summation formula to evaluate the summation over energy levels, but this method was open to the same objections as arise in the case of

classical statistics.

Peierls (1933, [3]) demonstrated how the dHvA effect is a direct consequence of the Fermi-Dirac statistics for the electrons. This statistics is in turn a consequence of Pauli exclusion principle for fermions. In the 1940s, dHvA oscillations were observed in many other metals.

In 1951, Sondheimer and Wilson [4] evaluated the grand canonical potential in the Fermi-Dirac statistics essentially by the inverse Laplace transform of the classical partition function, regarded as a function $Z_B(\beta)$ of $\beta = 1/k_B T$, where k_B is the Boltzmann constant and T is the absolute temperature. This mathematical method, which is rigorous for the free electron gas, can be applied to metals, only if the binding energy can be neglected. The binding can be taken into account by the effective mass m^* .

In 1952, Lars Onsager gave a physical explanation of the phenomenon, relating it to the Fermi surface of metals. In 1952, Dingle explained the amplitude reduction of oscillations through the broadening of the LL, caused by electron scattering by impurities. Starting from the 1960s, the dHvA effect was studied in two-dimensional electron gas (2DEG).

In the 1980s, the field of research of 2DEG systems in high magnetic fields and at low temperatures has brought to the discovery of superconducting side effects, as the integer and fractional quantum Hall effect (respectively von Klitzing, and Laughlin, 1985 and 1998 Nobel Prizes in physics).

The dHvA effect has been exploited to measure the Fermi surface (FS) of metals; this technique is still widely used for its precision: in 2009 only, more than 30 papers appeared on APJ journals, dealing with such s (for example [1, 5, 6, 7]).

1.3 The dHvA effect and the Fermi Surface

In two dimensions, the Fermi Energy corresponds to $E_F = \frac{N\hbar^2}{Am^*}$. The density of states at the Fermi Energy in two dimensions is

$$\rho(E_F) = \frac{Am^*}{\pi\hbar}$$

Notice that below the Fermi energy, at small T , the degeneracy of states g corresponds to the density ρ , for they are all occupied. There are many measurable quantities that contain information about the geometric structure of the Fermi surface. The knowledge of the shape of the Fermi surface allows to calculate the transport coefficients of the metal along with its equilibrium

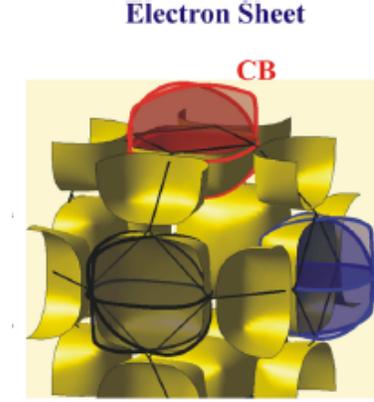


Figure 3: Fermi Surface for valence electrons of ZrB_{12} (Gasparov, 2008, [8])

and optical properties. The de Haas-van Alphen effect is the most powerful technique to deduce the geometry of the Fermi surface. In 1952, Onsager pointed out that the change in $1/H$ through a single period of oscillation was determined by the remarkably simple relation

$$\nu = \Delta \left(\frac{1}{H} \right) = \frac{2\pi e}{\hbar c} \frac{1}{A_{extr}}$$

A_{extr} is any extremal cross-sectional area A_{extr} of the Fermi surface (in k -space) in a plane normal to H . Altering the \vec{H} direction brings different extremal areas into play. All the A_{extr} of the Fermi surface can be mapped out. In real solids such a surface can be quite complex, Fig. (3). In a sense, measuring the frequency of the dHvA oscillations for different directions of the magnetic field is like making a tomography of the Fermi surface.

In the simpler case of free, non interacting electrons, in no magnetic field, the FS is just a sphere (or, in 2D, a circle) in the momentum-space. The quantization for the 3D case is depicted in Fig. (7).

2 Quantum mechanics

In non-relativistic theory, a magnetic field can be regarded only as an external field. The magnetic interactions between particles are a relativistic effect. Since electron speeds in a solid are small compared with the speed of light, Dirac relativistic equation reduces to the Schrödinger equation, which determines the time evolution of the system:

$$i\hbar\frac{d}{dt}\phi = \mathcal{H}\phi \quad (1)$$

where ϕ is the wavefunction of the system, and \mathcal{H} is the Hamiltonian operator, the extension to QM of the classical Hamiltonian function, which describes the energy of the system in terms of the canonical coordinates position and momentum.

We are interested in finding the eigenfunctions ψ of the Hamiltonian operator, in order to determine the eigenvalues of the energy E . Eq. 1 becomes:

$$\mathcal{H}\psi = E\psi \quad (2)$$

We shall consider the problem with two slightly different approaches. First, we find in an immediate way the eigenvalues E through *algebraic* considerations; secondly, we *solve the differential equation* to determine explicitly the energy eigenfunctions. Before doing so, we give a motivation to the quantum description of the problem.

Van Leeuwen theorem. Bohr (1911), and then Van Leeuwen (1919) pointed out how no magnetic effect can arise from a classical mechanical system at thermal equilibrium. Here we give an intuitive procedure to convincing of this result, anticipating some notions of statistical mechanics that are defined in section 3.

We calculate the free energy F of the system, which is the work that the system can do; then we use the thermodynamical relation

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

to calculate the magnetization. In classical mechanics, and using classical statistics,

$$F = -Nk_B T \log \iint dpdq e^{-\mathcal{H}(\vec{p}, \vec{q})/k_B T} \quad (3)$$

where

$$\mathcal{H}(\vec{p}, \vec{q}) = \frac{1}{2m} \left(\vec{p} + \frac{e}{c} \vec{A} \right)^2 \quad (4)$$

is the Hamiltonian of a charged, spinless electron in a magnetic field; the electron's charge is $-e$. We substitute as integration variable

$$\vec{\Pi} = \vec{p} + \frac{e}{c} \vec{A}$$

in place of the momentum \vec{p} , noting that $\frac{d\vec{p}}{d\vec{\Pi}} = 1$. We point out that the *canonical momentum* is \vec{p} , while $\vec{\Pi}$ is called the *kinetic momentum* $m\vec{v}$, which is defined by one of the two Hamilton equations

$$\frac{\vec{\Pi}}{m} = \dot{\vec{q}} = \frac{\partial \mathcal{H}}{\partial \vec{p}} \quad (5)$$

If in eq. (3) we perform the integration over $\vec{\Pi}$, it is at once evident that the vector potential \vec{A} , and with it the magnetic field \vec{H} , disappears from the equation. The free energy does not depend on the magnetic field, and therefore there is no magnetization, $M = \frac{\partial F}{\partial H} = 0$.

In quantum mechanics the observables \vec{A} and \vec{p} do not commute: $[\vec{A}, \vec{p}] \neq 0$; that is the reason why magnetic effects live up to the macroscopic level.

2.1 Landau levels

The Hamiltonian operator of a free, noninteracting electron in a magnetic field is

$$\mathcal{H} = \frac{1}{2m} \left(\vec{p} + \frac{e}{c} \vec{A} \right)^2 - \mu_B \vec{\sigma} \cdot \vec{B} \quad (6)$$

where $\nabla \times \vec{A} = \vec{B}$. From now on we make the approximation $\vec{B} = \vec{H} + 4\pi \vec{M} \approx \vec{H}$, where \vec{H} is the external magnetic field and \vec{B} is the induction field, that takes into the account the variation due to magnetization \vec{M} . In the situation in analysis this is a good approximation, as H is of some Tesla of magnitude.

The Hamiltonian is separable in two commuting terms

$$\mathcal{H} = \mathcal{H}_{//} + \mathcal{H}_{\perp} = \frac{p_z^2}{2m} + \mathcal{H}_{\perp}$$

where we have supposed that the field is in the \hat{z} direction, without a loss in generality. $\mathcal{H}_\perp = \frac{1}{2m}(\Pi_x^2 + \Pi_y^2)$, defining the canonical momentum $\vec{\Pi}$ as

$$\frac{\Pi_i}{m} = \dot{x}_i = \frac{1}{i\hbar}[\mathcal{H}, x_i] = (p_i + \frac{e}{c}A_i) \quad (7)$$

which is the quantum analogue of the classical Hamiltonian relation, eq. (5). From now on we substitute q_i with x_i . It is clear that the vector potential has no component in the the \hat{z} direction, both in the *symmetric gauge* $\vec{A} = \frac{1}{2}\vec{H} \times \vec{r}$, which in this case reduces to $\vec{A} = H/2 \begin{pmatrix} -\hat{y} \\ \hat{x} \\ 0 \end{pmatrix}$, and in

the *Landau gauge* $\vec{A} = H \begin{pmatrix} 0 \\ \hat{x} \\ 0 \end{pmatrix}$.

$$[\Pi_y, \Pi_x] = [p_y + \frac{e}{c}A_y, p_x + \frac{e}{c}A_x] = \frac{eH}{c}i\hbar$$

We notice that this commutation relation is similar to the canonical commutation relation that determines the position-momentum uncertainty. We define

$$\pi_i = \frac{\Pi_i}{\sqrt{eH/c}}$$

These operators satisfy the canonical commutation relations

$$[\pi_y, \pi_x] = i\hbar$$

We can rewrite the Hamiltonian as:

$$\mathcal{H}_\perp = \frac{1}{2} \frac{eH}{cm} (\pi_x^2 + \pi_y^2) = \frac{1}{2} \omega_c (\pi_x^2 + \pi_y^2) \quad (8)$$

where $\omega_c = eH/mc$ is the *cyclotron frequency*. In analogy with the theory of the 1D harmonic oscillator we now define the ladder operators,

$$a = \frac{\pi_y + i\pi_x}{\sqrt{2\hbar}} \quad a^\dagger = \frac{\pi_y - i\pi_x}{\sqrt{2\hbar}}$$

which bring the Hamiltonian in the standard form

$$\mathcal{H}_\perp = \hbar\omega_c(\hat{n} + \frac{1}{2}) \quad (9)$$

where $\hat{n} = a^\dagger a$ is the usual number operator.

The eigenvalues of the whole Hamiltonian are determined by the three quantum numbers k, n, m_s :

$$E_{k,n,m_s} = \frac{\hbar^2 k^2}{2m} + \hbar\omega_c \left(n + \frac{1}{2}\right) - \mu_B m_s H \quad (10)$$

$k \in \mathbb{R}$ is the \hat{z} component of momentum, $n = 0, 1, 2, \dots$ is the discrete energy value due the magnetic field, while $m_s = \pm 1$ depends on the spin, that can either be aligned in the direction of the field or opposite to it.

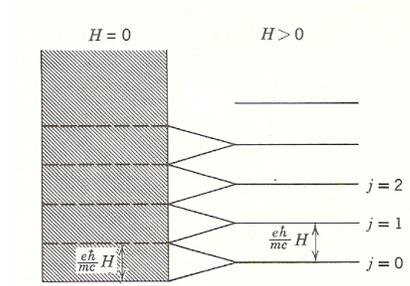


Figure 4: Energy spectrum, for $H = 0$ and $H > 0$.

These results are rigorous for noninteracting, non-relativistic electrons. In order to approximate the behaviour of conduction electrons in metals, we substitute m with an effective mass m^* that should take care of the adiabatic potential of the crystal V_{ad} , in a very rough approximation. The effective mass is properly a tensor, but in this simplified work we assume that $m_{ij}^* \equiv m^*$. This identity holds:

$$\frac{1}{2}\hbar\omega_c = \frac{m}{m^*}\mu_B H \quad (11)$$

where we recall that $\mu_B = e\hbar/2mc = 9.27 \cdot 10^{-24} J/T$ is the Bohr magneton.

Eigenfunctions. In order to find the eigenfunctions of E , it turns out to be convenient to work with the vector potential in the *Landau gauge* $\vec{A} = H \begin{pmatrix} 0 \\ \hat{x} \\ 0 \end{pmatrix}$. There is some freedom in the choice of vector potential for a

given magnetic field. However, the Schrödinger equation is gauge invariant, which means that adding the gradient of a scalar field χ to \vec{A} ,

$$\begin{aligned}\vec{A} &\rightarrow \vec{A} + \nabla\chi \\ \phi &\rightarrow e^{\frac{i}{\hbar}\chi}\phi\end{aligned}$$

changes the overall phase of the wave function by an amount corresponding to the scalar field so that $|\phi'|^2 = |\phi|^2$. Physical properties are not influenced by the specific choice of gauge.

We reconsider eq. (2):

$$\frac{\partial^2\psi}{\partial x^2} + \left(\frac{\partial}{\partial y} - \frac{ieHx}{\hbar c}\right)^2\psi + \frac{\partial^2\psi}{\partial z^2} = \frac{2mE}{\hbar^2}\psi \quad (12)$$

Since equation 12 contains neither y or z explicitly, we may assume $\psi(x, y, z) = e^{i(k_y y + k_z z)}u(x)$ and obtain for the function u the equation

$$u'' + \left\{ \frac{2mE_1}{\hbar^2} - \left(k_y - \frac{eH}{\hbar c}x\right)^2 \right\} u = 0 \quad (13)$$

where $E_1 = E - \frac{\hbar^2}{2m}k_z^2$ is the energy of the motion in the transverse plane. Eq.(13) is the differential equation of a one-dimensional harmonic oscillator with frequency $\frac{eH}{mc} = \omega_c$ and center $x_0 = \frac{\hbar c}{eH}k_y$, which is called the *guiding center*.

To find the number of states belonging to each energy eigenvalue, we have to specify the *boundary conditions*. In the y-direction and z-direction we shall assume the cyclic condition, which allows values for k_y and k_z that are multiples of $2\pi/L_y$ $2\pi/L_z$ respectively. We choose to enforce the cyclic condition in the y-direction only. However, B. I. Halperin showed that it is possible to obtain a periodic solution in x and y.

We assume, instead, that in the x-direction the system is bounded by two walls, a distance L_x apart. If the L_x is large compared to the extension of the oscillator function $u_n(x - x_0)$, which is of the order of the orbital radius, the functions for which the center x_0 lies well inside the volume will not be affected by the presence of the walls. This solutions correspond to the *bulk states*, and form the typical discrete energy levels that you can see in Fig. (5). No solutions exist if x_0 lies well outside the volume; for a small range of x_0 near the wall, the presence of the wall modifies the oscillator eigenfunction,

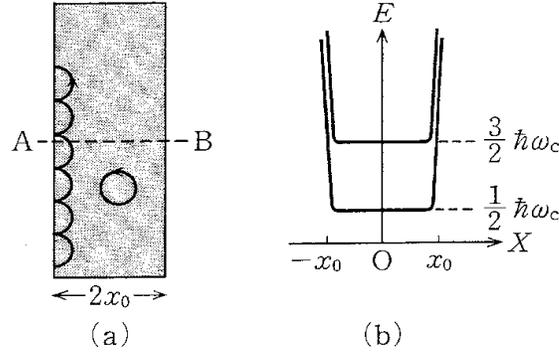


Figure 5: (a) semi-classical orbits of electrons in the plane normal to B. (b) Landau Levels at the edge of the sample [23].

determining the steep slope in correspondence to the walls. The permissible interval of k_y is $L_x eH / \hbar c$.

There are

$$g = \frac{L_x L_y eH}{2\pi \hbar c} = \frac{A}{2\pi l^2} \quad (14)$$

states of the same energy.

$$l = \sqrt{\frac{\hbar c}{eH}} \quad (15)$$

l is the *magnetic length*, g is the *degeneracy* of each Landau Level, which is to be multiplied by the $g_s = 2$ degeneracy due to spin only if we neglect the spin split in energy. The ratio between the separation of Landau levels $\hbar \omega_c$ and the Zeeman split $2\mu_B H$ is m^*/m , which is negligible, m^* being some percent of the bare mass m . For a field of 1 Tesla and a strip of 1 mm sides the degeneracy is of the order of 10^{10} .

Now, we consider the two-dimensional problem, suppressing motion in the z direction, reducing it to a strip of sizes L_x and L_y . We impose periodic boundary conditions in y . We simplify the notation of eq. (13), normalize the variables, $x/l \rightarrow \xi$ so to obtain Weber's equation:

$$-\psi''(\xi) + (\xi - \xi_0)^2 \psi(\xi) = \epsilon \psi(\xi) \quad (16)$$

whose general solution is a linear combination of Parabolic Cylinder func-

tions:

$$\psi_{k,p}(\xi) = AD_n(\sqrt{2}(\xi - \xi_0)) + BD_n(-\sqrt{2}(\xi - \xi_0)) \quad (17)$$

The real parameters A, B and $n = (\epsilon - 1)/2$ (n can take also rational values!) are constrained by the boundary conditions $\psi = 0$ at the edges, and by normalization $1 = \int_0^{L_x/l} d\xi |\psi(\xi)|^2$. For a fixed value of ξ_0 , the solutions are orthogonal and correspond to a sequence of discrete eigenvalues. Each eigenvalue, regarded as a function of ξ_0 , is a *Landau branch*.

Bulk and edge states. Weber's solutions can be divided in bulk states and edge states. For bulk states each branch n is a straight horizontal line, and there is no dependence on the center of the orbit ξ_0 ; the branches are equally spaced. The corresponding eigenfunctions are those of the 1D harmonic quantum oscillator, for which:

$$\psi_{k,n}(\xi) = \frac{1}{\sqrt{\sqrt{\pi}2^n n!}} e^{-\frac{1}{2}(\xi - \xi_0)^2} H_n(\xi - \xi_0) \quad (18)$$

The eigenvalue is $\epsilon_n = 2n + 1$ with integer n , and H_n are the Hermite polynomials,

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2} \quad (19)$$

Determining the exact solution of the wavefunctions near the edge is a complex task; recently Wang *et al.* (2009, [7]) gave an accurate treatment of the problem, though numerical methods, including the spin-orbit interaction that in real metals further splits spin-up and spin-down levels, Fig. (6).

The edge states, as visible in fig. (5), have eigenvalues that tend to infinity as the center of orbit ξ_0 tends to the wall. We may account for this with two simple and just qualitative arguments. The first one is that, in a semi-classical frame, the electron does not close the circular orbit, instead it keeps bouncing on the edge, shifting of a length r_s - upwards if it is next to the right edge, downwards if it is at the left edge. This is a very intuitive explanation of how two opposite currents build up at the edges of a 2DEG sample, and further investigation leads to understanding the arising of the integer quantum Hall effect.

Another insight involves Heisenberg's uncertainty principle, $\Delta x \Delta p \geq \hbar/2$. We can imagine the contribution of an eigenvalue $\epsilon(\xi)$ for which the guiding center $\xi_0 \gg L_x/l$ is well outside the sample, say at the foremost right; it shows a parabolic behaviour, and it intersects the infinite wall of the edge

at higher and higher energies as the guiding center is shifted farther from the wall. This implies a narrower spatial range Δx in which the electronic wavefunction is localized; as a backlash, momentum, and thus energy, gets higher and higher.

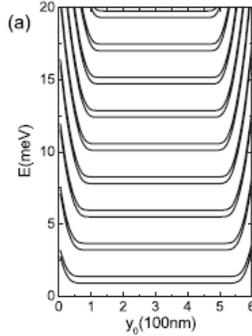


Figure 6: The energy spectrum in units of meV versus the guiding center, here called y_0 . Through numerical methods, Wang 2009 [7].

Eventually, we notice that the choice of the symmetric gauge would lead to a different study of the solutions of the differential equation; we just point out that in that representation the eigenfunctions of energy are also eigenfunctions $\psi(r)$ of the angular momentum z -component, L_z , thus embodying the symmetry of the system under rotation around the z axis. Indeed, the high degeneracy of the Landau Levels reflects this multiple symmetries of the system. In the Landau gauge it's evident the invariance under translational displacement, at least for bulk states. Below, we give a further insight to the meaning of degeneracy.

Flux quantization. The total magnetic flux passing through the sample is

$$\Psi = \int \vec{H} \cdot \vec{n} da = H \int da = HL_xL_y \quad (20)$$

so that we can express the degeneracy from eq. (14) as

$$g = \frac{L_xL_yHe}{2\pi\hbar c} = \frac{\Psi e}{2\pi\hbar c} \equiv \frac{\Psi}{\Psi_0} \quad (21)$$

where $\Psi_0 = \hbar c 2\pi / e$ can be viewed as the flux quantum. It is noteworthy to say that this simple derivation finds an analogue in the quanta of flux generated by the electronic vortices in superconductors - with charge $2e$ because electrons are paired.

The qualitative fact is that the flux quantization sets a finite minimum size of an orbit and thereby provides the escape from Van Leeuwen theorem.

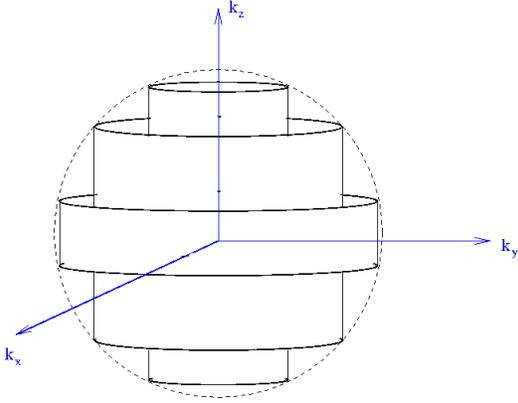


Figure 7: The plot of points in (k_x, k_y, k_z) -space. The dotted sphere represents the Fermi energy surface. Graphics from Lahiri, [14].

2.2 The dHvA effect

We give a qualitative and intuitive insight of the phenomenon, following Huang [9].

The Landau Levels are the discrete eq. (10). The degeneracy g is linear in H (strength of the magnetic field), eq. (14). At low T , electrons occupy the lowest available energy levels; since the levels below the Fermi energy are all filled (only the last level can be partially filled), the degeneracy corresponds to the density of states. At N fixed, decreasing the field H provokes g to decrease, and fewer electrons can be accommodated on each level. Some electrons will be forced to jump to a higher energy level. This causes the low- T oscillation of magnetic susceptibility as H is decreased.

Ashcroft [5] points out that the level density will have a sharp peak whenever

E is equal to the energy of an extremal orbit satisfying the quantization condition $\Delta A = \frac{2\pi e}{\hbar c} H$. The sets of orbits satisfying the condition for a given n form a tubular structure in k -space, Fig. (7). Most electronic properties of metals depend on the density of states at the Fermi energy, and $g(E_F) = \rho(E_F)$ will be singular whenever H causes an extremal orbit on the FS to satisfy the quantization condition. $\rho(E_F)$ is singular at regularly spaced intervals in $1/H$ given by

$$\nu(dHvA) = \Delta \left(\frac{1}{H} \right) = \frac{2\pi e}{\hbar c} \frac{1}{A_{extr}} \quad (22)$$

The dHVA effect can be observed in very pure metals only at low temperatures and in strong magnetic fields that satisfy

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

Thus the oscillatory behaviour as a function of $1/H$ should appear in any quantity that depends on the level density at E_F - which, at $T = 0$, includes almost all characteristic metallic properties. The oscillating behaviour is not detectable if $k_B T$ is greater than the spacing between the LL, $k_B T \gg \hbar\omega_c$. Electron scattering constitutes another problem, and the electronic relaxation time τ provides a limit in the definition of energy, as for the time-energy uncertainty principle, $\Delta E \approx \hbar/\tau$.

3 Statistical mechanics

Statistical mechanics provides the connection between mechanics (quantum, or classical) and thermodynamics, which accounts for heat, temperature and other macroscopic quantities of many-particles systems - in the simplest case: a noninteracting gas. We will treat here only equilibrium thermodynamics, that is, all macroscopic quantities have reached the mean value and there are no fluctuations. Van Leeuwen's theorem states that no magnetic effect can be generated by a classical system at thermal equilibrium. For this reason we will start with a quantum mechanical description of the Hamiltonian, considering the case of the previous section: electrons in a magnetic field.

The second law of thermodynamics states that thermodynamic equilibrium is reached when entropy is maximal for constant internal energy U . It is easy to see that this is equivalent to requiring a minimum of internal energy for constant entropy. (If the internal energy were not minimal, we could extract work and then re-inject it in the form of heat, thereby increasing the entropy). In practice, it is usually the temperature which is kept constant. We must re-express the second law in terms of the minimum of a new thermodynamic function. This will be done explicitly below, by carrying out a Legendre transformation. This function is the free energy:

$$F = U - TS$$

in the case of a canonical ensemble, and is the grand canonical potential in the case of a varying number of particle N :

$$\Omega = F - \mu N \tag{23}$$

When the number of particles in the system is not fixed, it is then useful to specify the mean number of electrons by means of a chemical potential μ .

In differential form these definitions become

$$dF = HdM - SdT \quad d\Omega = dF - Nd\mu$$

3.1 Classical statistics

In classical statistical mechanics we use Boltzmann distribution to determine the probability of a given particle of the system at temperature $k_B T = 1/\beta$

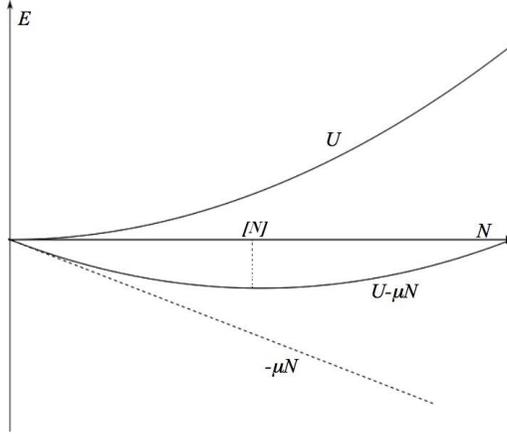


Figure 8: A sketch of internal energy U and free energy $F = U - \mu N$ versus N , the number of particles. It is evident that deriving F by the minus chemical potential μ gives the statistical mean number of particles at equilibrium $[N]$

to be at energy E is given just by $p(E) = \frac{1}{Z} e^{-\beta E}$. Z is the normalizing factor, called *partition function*, since $\sum_{\alpha} p_{\alpha} = 1$ for the possible α energy states. Z retains all the thermodynamical information of the system, which can be calculated through partial derivation.

$$Z_B(\beta) = \sum_{\alpha} g(E_{\alpha}) e^{-\beta E_{\alpha}} \quad (24)$$

In our case,

$$Z = \int dpdq e^{-\beta \sum_i H_i(p,q)} = \int dpdq e^{-\beta \sum_i \frac{1}{2m} (\vec{p}_i + \frac{e}{c} \vec{A}(\vec{q}_i))^2} \quad (25)$$

From now on $|\vec{H}| = H$ is the strength of the field, not to be confused with the Hamiltonian operator, \mathcal{H} . If the electrons were not subject to Pauli principle, the Boltzmann statistics for thermal equilibrium would apply (we denote it by Z_B):

$$Z_B(\beta, H) = \sum_{k,n,m_s} g(E) e^{-\beta E_{k,n,m_s}} \quad (26)$$

where the eigenvalues follow equation (10) and the degeneracy of each energy level is given by eq. (14). Every part of the Hamiltonian commutes with the others, since k is for the translational degrees of freedom, n for the interaction

of the orbital magnetic moment and the field, and m_s for the internal degree of freedom represented by the spin-field interaction. The relative partition function is thus separable - it is the product of its different parts:

$$Z_B(\beta, H) = Z_{tr}(k)Z_{LL}(n)Z_s(m_s)$$

where $E_k = \frac{p_x^2}{2m} = \hbar^2 k^2 / 2m$. If the particle is confined in the x -direction in a strip of size $L_x = L$, we can take the periodic boundary conditions so that the wavefunction is the same at opposite boundaries:

$$E_k = \frac{\hbar^2 k^2}{2m}, \quad k = \frac{2\pi}{L}n, \quad n \in \mathbb{Z}$$

in the limit of macroscopically large L , the plane wave states form a continuum, so that we can approximate the sum for the partition function by the Gaussian integral

$$Z_{tr} = \sum_k e^{-\beta E_k} \approx \int_{-\infty}^{\infty} e^{-\beta \frac{(2\pi\hbar)^2 x^2}{2mL^2}} dx$$

We can then simplify the equation since the latter is the Gaussian integral:

$$Z_{tr} = \frac{L}{\Lambda}, \quad \Lambda = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}$$

where we have introduced the *thermal length* Λ .

The product of the three partition functions becomes:

$$\begin{aligned} Z_B(\beta, H) &= \sum_{k,n,m_s} g(E) e^{-\beta E_{k,n,m_s}} \\ &= g Z_{tr} \sum_n e^{-\beta \hbar \omega_c (n + \frac{1}{2})} \sum_{m_s} e^{\beta \mu_B m_s H} \\ &= \frac{A}{2\pi l^2} \frac{L}{\Lambda} \exp\left(\frac{-\beta \hbar \omega_c}{2}\right) \sum_{n=0}^{\infty} (e^{-\beta \hbar \omega_c})^n \sum_{m_s=-1,+1} e^{\beta \mu_B m_s H} \end{aligned} \tag{27}$$

$$= \frac{V}{\Lambda 2\pi l^2} \frac{\cosh(\beta \mu_B H)}{\sinh(\beta \hbar \omega_c / 2)} \tag{28}$$

3.2 Quantum statistics

Here we account for the effects of quantum mechanics on the distribution of the particles (or, if you prefer, of the *wavefunctions*) of the system. There is a double presence of QM, both in the Hamiltonian operator (and in the redefinition of the underlying mathematics), and in the resulting statistics for low temperatures. That is the regime in which the condition on the symmetry or antisymmetry of the wavefunction makes the Bose-Einstein or the Fermi-Dirac distributions emerge, respectively for bosons or fermions. The latter is called Pauli's exclusion principle, for no more than two electrons can occupy the same energy level.

In QM, particles are either fermions or bosons, depending on their behaviour under inversion of parity of their wavefunction (for a more precise explanation, see any basic QM textbook, as [12]). Bosons, which are characterized by a totally symmetric wavefunction, behave in a "social-like" way, being possible to push as many of them on any energy level. On the contrary, the antisymmetrized wavefunctions of fermions imply that at most two of them can occupy the same energy level, the factor 2 brought in by the possible orientation of the spin. Thus fermions show up as an "incompressible" fluid, since the exclusion principle produces a repulsion between particles.

We now analyze how this peculiar quantum effect determines radically different behaviour on the macroscopic level. The grand partition function is:

$$Q = \prod_{\alpha} \left[\sum_n (e^{\beta(\mu - E_{\alpha})})^n \right] \quad (29)$$

The sum in brackets can be carried out explicitly: for fermions $n = 0, 1$, thus it equals $1 + e^{\beta(\mu - E_{\alpha})}$; for bosons, $n = 0, 1, 2, \dots$, therefore that sum is a geometric series, whose summation gives $(1 - e^{\beta(\mu - E_{\alpha})})^{-1}$. In a compact mode, we can rewrite the grand canonical partition function as:

$$Q = \prod_{\alpha} [e^{\beta(\mu - E_{\alpha})}]^{-\theta}$$

where $\theta = +1$ for bosons and $\theta = -1$ for fermions. From now on we shall disregard the boson case, as we deal with electrons, which are fermions. We can define the mean occupation number, known as the *Fermi function* as

$$n(E) = f(E) = \frac{1}{1 + e^{\beta(E - \mu)}} \quad (30)$$

One of the most relevant thermodynamical potentials for grand canonical ensembles is the grand canonical potential, that for fermions is

$$\Omega = -PV = -k_B T \log Q = -k_B T \sum_{\alpha} \log(1 + e^{\beta(\mu - E_{\alpha})}) \quad (31)$$

At $T = 0$ it is possible to approximate this summation by the Poisson summation formula, first used for this purpose by Landau(1938), or by the Euler Maclaurin formula, which was used for the calculation of the steady diamagnetism (also by Landau, 1930). The two methods differ essentially only in that the Fourier analysis is put in at the start in the Poisson approach and at the end in the Euler-Maclaurin one (for a complete derivation see *Shoenberg* [1]), in Appendix 3 and sec 2.3.1.

3.3 Peierls' method

In the next two sections we will use Peierls' method to evaluate the grand canonical potential Ω essentially via a Laplace inverse transform of the Boltzmann partition function Z_B . This method provides a useful connection between a canonical and a grand canonical description of the ensemble, through exact and simple calculations.

We should point out how a grand canonical description of the system (which leaves not fixed the energy E , nor the number of particles N) is the most suitable for quantum mechanics, not only because it allows to ease the sum over the levels of energy (which becomes a convergent series), but also for it embodies the Principle of indetermination: at any given moment, it is not possible to know exactly how many electrons compose the system. Moreover, from a more practical perspective, we shall observe that wires, and metallic surfaces in general, provide an almost ideal reservoir of electrons.

We derive the *grand canonical* potential Ω from the *canonical* partition function, instead that from the grand canonical partition function Q of eq. (31).

Proposition

$$\Omega = \int_0^{\infty} dE z(E) \frac{\partial f(E)}{\partial E} \quad (32)$$

$$z(E) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{sE} \frac{Z_B(s)}{s^2} \quad (33)$$

where s is the extension of β to the complex plane, $c \in \mathbb{R}$, $c \geq 0$ and

$$f(E) = \frac{1}{e^{\beta(E-\mu)} + 1}$$

is the Fermi occupation number of a state of energy E , defined in eq. (30). A proof of the proposition is given in the Appendix (§A.2).

3.3.1 Peierls' method for the electron gas in 3D

We apply Peierls' method in the case of the 3D electron gas in no magnetic field.

$$Z_B = g_s \sum_{k,n,m_s} e^{-\beta \frac{\hbar^2 k^2}{2m}} = 2 \left(\frac{L}{\Lambda} \right)^3 = 2V \left(\frac{m}{2\pi\hbar^2\beta} \right)^{\frac{3}{2}} \quad (34)$$

we now extend $\beta \rightarrow s$ to a complex variable; equation 33 becomes

$$z(E) = 2V \left(\frac{m}{2\pi\hbar^2} \right)^{\frac{3}{2}} E^{5/2} \int_{c/E-i\infty}^{c/E+i\infty} \frac{ds}{2\pi i} e^s s^{-7/2}$$

If we apply the residue theorem to the integral above, we see that the relevant contribution comes only from the path on σ , Fig. (14), due to the negative-real axis branch cut. We notice that $\int_{\sigma} \frac{ds}{2\pi i} e^s s^{-7/2}$ is just Hankel's representation of the Gamma function (see Appendix A.4).

$$z(E) = \frac{2V}{\Gamma(7/2)} \left(\frac{m}{2\pi\hbar^2} \right)^{\frac{3}{2}} E^{5/2} = \alpha_0 E^{5/2}$$

we have introduced the constant α_0 , independent from the energy. The grand canonical potential is

$$\Omega_0 = \alpha_0 \int_0^{\infty} dE E^{5/2} f'(E)$$

For $\beta\mu \gg 1$, $f(E)$ is the ‘‘step function’’, also known as the *Heaviside function*, with step at $E = \mu$. Its derivative is Dirac delta function $-\delta(\mu - E)$, and the integration above is trivial:

$$f(E)_{T=0} = \begin{cases} 1 & E \leq \mu \\ 0 & E > \mu \end{cases}$$

$$\Omega_0 = -\alpha_0 \int_0^{\infty} dE E^{5/2} \delta(\mu - E) = -\alpha_0 \mu^{5/2} = -\frac{16}{15\sqrt{\pi}} V \left(\frac{m}{2\pi\hbar^2} \right)^{3/2} \mu^{5/2} \quad (35)$$

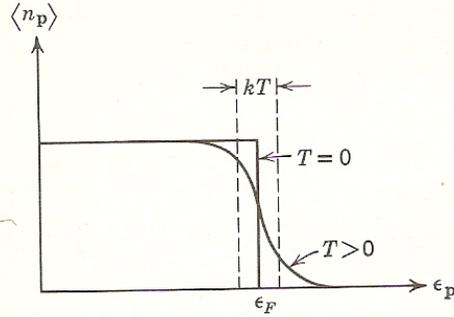


Figure 9: The Fermi function at $T = 0$ and T greater than 0. From Huang, [9].

3.3.2 Peierls' method in 2D for $\mathbf{H} = 0$

The Boltzmann canonical partition function, for an electronic gas in two dimensions (2DEG) is:

$$Z_B = g_s \sum_{\mathbf{k}} e^{-\beta \frac{\hbar^2 k^2}{2m}} = 2 \left(\frac{L}{\Lambda} \right)^2 = \frac{Am}{\pi \hbar^2 \beta} \quad (36)$$

Again, we evaluate the grand canonical potential through Peierls' method, according to equations (32), (33). We extend β to the complex plane and dub it s :

$$z(E) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{sE} \frac{Z_B(s)}{s^2} \quad (37)$$

$$= \frac{2A}{m2\pi\hbar^2} \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{sE} s^{-3} \quad (38)$$

$$= \frac{2A}{m2\pi\hbar^2} E^2 \text{Res}_0(e^z z^{-3}) = \frac{2A}{m2\pi\hbar^2} \frac{E^2}{2} \quad (39)$$

where we have applied the residues theorem, to the contour of Fig. (11); we made the change $sE \rightarrow z$ and evaluated the residue of $e^z z^{-3}$ due to the pole of order III in $z = 0$. The residue is equal to the a_{-1} coefficient of the Laurent series $f(z) = \sum_{-\infty}^{+\infty} a_n z^n$.

It follows:

$$\Omega_0^{2D} = \frac{2A}{2\pi\hbar^2} m \int_0^\infty dE E^2 f'(E)$$

For $\beta\mu \gg 1$, $f(E)$ is the “step function”, also known as *Heaviside function*, with step at $E = \mu$. Its derivative is the Dirac delta function $-\delta(\mu - E)$, and the integration above is trivial:

$$\Omega_0^{2D} = -\frac{Am}{4\pi\hbar^2}\mu^2 \quad (40)$$

4 3D system

We apply Peierls' method to find the overall magnetization of the electronic gas confined in a cubic box.

As Sondheimer and Wilson pointed out in their 1951 article: “*The inverse Laplace transform of Z_B has a simple physical meaning: it is the number of energy levels per unit energy interval*” [4].

In the problem considered here, both in 3D and 2D (next section), Z_B is a complicated oscillatory function of the energy, whereas its Laplace inverse transform is a simple monotonic function.

We consider $Z_B(s)$, where s is the extension of β to the complex plane. The behaviour of the inverse Laplace transform of $Z_B(\beta)$ is determined by its singularities. The branch cut on the negative-real axis gives the steady diamagnetism, including its point variation with T and H , while the poles at $s = in\pi$ produce the dHvA oscillations.

It is necessary to account for the electron spin interaction with the external field H , which introduces a paramagnetic effect that adds to the total susceptibility.

If two terms of the Hamiltonian commute, the relative partition function is separable: $Z_B = Z_L \cdot Z_P$, Z_B divides into Landau's and Pauli's factors.

For independent electrons in a magnetic field, eq. (33) is:

$$z(E) = 2V \left(\frac{m^*}{2\pi\hbar^2} \right)^{\frac{3}{2}} \left(\frac{\hbar\omega_c}{2} \right)^{\frac{5}{2}} \mathcal{I}\left(\frac{2E}{\hbar\omega_c}\right) \quad (41)$$

$$\mathcal{I}(x) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{sx} \frac{\cosh(sm^*/m)}{s^{5/2} \sinh s} \quad (42)$$

A. Landau and Pauli susceptibilities. The integral along σ gives a contribution which can be evaluated approximating the singular behaviour of the integrand in the origin: $s^{-5/2}(\sinh s^{-1}) = s^{-7/2} - \frac{1}{6}s^{-3/2} + R(s)$. The

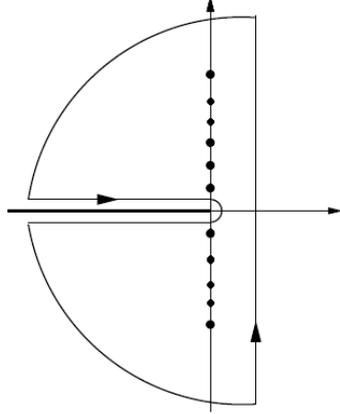


Figure 10: The path $(c - i\infty, c + i\infty)$ in the complex s -plane is completed in the oriented contour C that avoids the cut $\text{Res} < 0$ and encloses simple poles on the imaginary axis. While the two arcs do not contribute to the integral, the integral on the path $(-\infty + i\epsilon, -\infty - i\epsilon)$ enclosing the cut does, and is subtracted (added with orientation reversed: this is path σ).

remainder R is just the different and is finite in $s = 0$.

$$\begin{aligned}
 \mathcal{I}_\sigma(x) &= \int_\sigma \frac{ds}{2\pi i} e^{sx} \frac{\cosh(sm^*/m)}{s^{5/2} \sinh s} & (43) \\
 &= \frac{1}{2} \left[\left(x + \frac{m^*}{m}\right)^{5/2} + \left(x - \frac{m^*}{m}\right)^{5/2} \right] \int_\sigma \frac{ds}{2\pi i} e^s s^{-7/2} \\
 &\quad - \frac{1}{12} \left[\left(x + \frac{m^*}{m}\right)^{1/2} + \left(x - \frac{m^*}{m}\right)^{1/2} \right] \int_\sigma \frac{ds}{2\pi i} e^s s^{-3/2} \\
 &\quad + \int_\sigma \frac{ds}{2\pi i} e^{sx} \cosh\left(s \frac{m^*}{m}\right) R(s) & (44)
 \end{aligned}$$

where the first two integrals are Hankel's representation of the Gamma function (see Appendix A.4, eq. (79)). The integral thus reduces to:

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

At $T = 0$ it is $f'(E) = -\delta(\mu - E)$ and the integration is trivial

$$\Omega_{PL} = -2V \left(\frac{m^*}{2\pi\hbar^2} \right)^{3/2} \left(\frac{\hbar\omega_c}{2} \right)^{5/2} \mathcal{I}_\sigma\left(\frac{2\mu}{\hbar\omega_c}\right) \quad (45)$$

and for small magnetic field ($\mu \gg \hbar\omega_c$) the large x expansion is used up to $\mathcal{O}(H^2)$,

$$= \Omega_0 - \frac{2}{\sqrt{\pi}} V \mu_B^2 H^2 \mu^{1/2} \left(\frac{m^*}{2\pi\hbar^2} \right)^{3/2} \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] \quad (46)$$

where Ω_0 is the partition function of the Fermi gas in zero field and $T = 0$. $M = -\partial\Omega/\partial H$. The correction to μ for E_F is quadratic in H , so we can replace μ with E_F in the expression for M . At fixed density, it yields the magnetic susceptibility per unit volume:

$$\begin{aligned} \chi &= \frac{1}{V} \left(\frac{\partial M}{\partial H} \right)_{N,V} \\ &= \frac{4}{\sqrt{\pi}} \mu_B^2 \sqrt{E_F} \left(\frac{m^*}{2\pi\hbar^2} \right)^{3/2} \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] \\ &= \mu_B^2 \rho(E_F) \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] \end{aligned} \quad (47)$$

$$(48)$$

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

B. dHvA oscillations. The contour integral is evaluated exactly by summation of residues in $s = \pm in\pi$, $n = 0$ is excluded by the contour:

$$\mathcal{I}(x) = \int_C \frac{ds}{2\pi i} e^{sx} \frac{\cosh(sm^*/m)}{s^{5/2} \sinh s} \quad (49)$$

$$= \sum_{n \neq 0} e^{inx} \frac{\cos(n\pi m^*/m)}{(in\pi)^{5/2}} \quad (50)$$

$$= -2 \sum_{n=1}^{\infty} \frac{(-1)^n}{(n\pi)^{5/2}} \cos(n\pi x - \frac{\pi}{4}) \cos(n\pi m^*/m) \quad (51)$$

where the mathematical passages are analyzed in the similar calculus for the dHvA oscillations in the 2D case. The relevant integral for Ω_{osc} is

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

for small temperatures the lower limit is taken to $-\infty$ and the integral is known (GR 3.982 [17])

$$\begin{aligned}
&= -\frac{1}{2} \cos\left(2n\pi \frac{\mu}{\hbar\omega_c} - \frac{\pi}{4}\right) \int_{-\infty}^\infty dt \frac{\cos\left(\frac{4n\pi}{\beta\hbar\omega_c} t\right)}{\cosh^2 t} \\
&= -\frac{2n\pi^2 \cos\left(2n\pi \frac{\mu}{\hbar\omega_c} - \frac{\pi}{4}\right)}{\beta\hbar\omega_c \sinh\left(\frac{2n\pi^2}{\beta\hbar\omega_c}\right)} \tag{52}
\end{aligned}$$

so that the contribution to the grand canonical potential produced by the summation on the simple poles of the imaginary axis is

$$\Omega_{osc} = \frac{V}{2\pi^2} k_B T \left(\frac{eH}{4\hbar c}\right)^{3/2} \sum_{n=1}^\infty \frac{(-1)^n}{(n)^{3/2}} \cos\left(\frac{n\pi m^*}{m}\right) \frac{\cos\left(2n\pi \frac{\mu}{\hbar\omega_c} - \frac{\pi}{4}\right)}{\sinh\left(\frac{2n\pi^2}{\beta\hbar\omega_c}\right)} \tag{53}$$

The Fermi surface in 3D. We shall determine the magnetization and magnetic susceptibility

$$\begin{aligned}
\Omega &= F - \mu N \\
M &= - \left(\frac{\partial \Omega}{\partial H}\right)_N \quad \chi = \frac{1}{V} \left(\frac{\partial M}{\partial H}\right)_{N,V}
\end{aligned}$$

but we need to do it at constant N and V :

$$\Omega(\mu, T, H) \rightarrow \tilde{\Omega}(N, T, H) \tag{54}$$

so that, first we evaluate N :

$$N = - \left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V}$$

and then we express the chemical potential μ as a function of N . Moreover: we make the identity $\mu \equiv E_F$ that is true for $T = 0$, for E_F is a meaningful constant.

5 2D system

We now consider a 2D system electron gas (2DEG). As for Hisihara [20], a given system is two dimensional if the characteristic length $\sqrt{D\tau_i}$ is larger than its thickness, where D is the diffusion constant and τ_i is the inelastic scattering time. In real applications, we can realize two-dimensional electron systems at interfaces between semiconductors [18].

Today, very clean AlGaAs-GaAs heterostructures constitute an almost perfect realization of a 2DEG [22]. Measuring the weak magnetization of dHvA oscillations represents a challenging experimental task. It is usually measured by torque magnetometers (magnetic torque $|\vec{\tau}| = |\vec{M} \times \vec{H}|$) as you can see from the experimental plot of Fig. (2). Other devices include torsional magnetometers with optical angular detection, micromechanical cantilever magnetometers, dc superconducting quantum interference device magnetometers [7].

We assume that the free electrons are bound to move in a plane, transverse to the direction of the magnetic field \vec{H} . As before, we assume that the field is uniform in space, and choose it in the z -direction; the electrons are in a x - y plane.

In a classical and semi-classical picture, in a 3D system, electrons in a magnetic field move in spirals, aligned on the field direction. In a 2D system their orbits just draw circumferences.

The energy E of the 3D system is continuous - the LL are discrete, but there is no quantization in the z -component of momentum, which remains unaffected by the field; in a 2D system though, the energy is completely discrete. Fujita *et al.* (2002) claim that a 2D system is intrinsically paramagnetic, since from their calculations Landau's diamagnetic term is absent; nevertheless they claim that the system exhibits dHvA oscillations [21]. We shall make the analytic calculations and partially overthrow this conclusion, since paramagnetism, diamagnetism, and dHvA oscillations all appear.

The Hamiltonian of an electron in a 2DEG sample is

$$\mathcal{H} = \hbar\omega_c(\hat{n} + \frac{1}{2}) - \mu_B \vec{\sigma} \cdot \vec{H} \quad (55)$$

where from the 3D system eq. (10) the k_z term is dropped. The eigenvalues are

$$E_{n,m_s} = \hbar\omega_c(n + \frac{1}{2}) - \mu_B m_s H \quad (56)$$

As before, we use Peierls' method to derive the grand canonical potential Ω from Boltzmann partition function Z . Then we evaluate the susceptibility χ through the thermodynamical relations:

$$M = -\frac{\partial\Omega}{\partial H}, \quad \chi = \frac{1}{V} \frac{\partial M}{\partial H} = -\frac{1}{V} \frac{\partial^2\Omega}{\partial H^2}$$

From the 3D Boltzmann partition function, the term $Z_{tr} = L/\Lambda$ is dropped, because motion in the z direction is suppressed; the partition function is then:

$$Z_B = \sum_{n,m_s} g(E) e^{-\beta E_{n,m_s}} = \frac{A}{2\pi l^2} \frac{\cosh(\beta\mu_B H)}{\sinh(\beta\hbar\omega_c/2)} \quad (57)$$

In order to get Ω from eq. (32), we need $z(E)$ from eq. (33); thus we calculate

$$z(E) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{sE} \frac{Z_B(s)}{s^2} = \frac{A}{2\pi\hbar^2} \frac{\hbar\omega_c}{2} \mathcal{I}(x)$$

where we have extended $\beta \rightarrow s'$ to the complex plane, and then $s' \rightarrow s2/\hbar\omega_c$. We have introduced

$$\mathcal{I}(x) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{sx} \frac{\cosh(sm^*/m)}{s^2 \sinh s} \quad (58)$$

In the last passage we have used the condition on the effective mass (eq. 11), setting $x = 2E/\hbar\omega_c$.

5.1 Calculating the integral

We use the residue theorem to calculate the integral above, closing the path of integration as shown in Fig. (11).

In this case, $\gamma = C(\alpha) + D(\alpha)$ where the path of integration in eq. (58) can be seen as $C = (c - i\infty, c + i\infty) = \lim_{\alpha \rightarrow \infty} [c - i\alpha, c + i\alpha]$ where D is the semicircle of radius $|\alpha|$ centered in c , towards the negative-real axis.

Hence if we call $f(s)$ the integrand in eq. (58), we see that it has infinite simple poles in $s = \pm in\pi$ due to the singular behaviour of $\sinh s^{-1}$ there, and a pole of order III in $s = 0$ as $\lim_{s \rightarrow 0} f(s) \approx s^{-3}$.

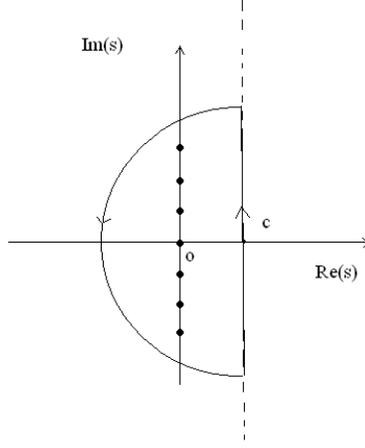


Figure 11: Integration in the 2D case. The singularities are one pole of order III in the origin and infinite simple poles on the imaginary axis at $\pm n\pi i$, with n any integer number. Note the difference from the 3D case: there is no branch cut on the negative-real axis, thus no need for the path σ .

For $\Re(s) \leq c$ the integrand is bounded and tends to zero on D because of the $s^{-2}e^{sE}$ factor. We can thus evaluate the integral in eq. (58):

$$\begin{aligned} \sum_n Res_{z_n}(f) &= \int_{\gamma} f(s) = \lim_{\alpha \rightarrow \infty} \left[\int_{C(\alpha)} f(s) + \int_{D(\alpha)} f(s) \right] \\ &= \int_C f(s) = 2\pi i \sum_{n \in \mathbb{Z}} Res_{n\pi i} f \\ \mathcal{I}(x) &= \mathcal{I}_0 + \mathcal{I}_{osc} \end{aligned}$$

First we evaluate the residue in the origin, then those on the imaginary axis.

1. The residue in $s = 0$ The residue in $s = 0$ is equal to the a_{-1} term of the Laurent series of f , that is $\sum_{-\infty}^{\infty} a_n s^n$. We can Taylor expand all the simple functions, which are all well-known series, and then multiply the terms. The Laurent series of $\frac{1}{\sinh(s)}$ is $(\frac{1}{s} - \frac{s}{6} + \frac{7}{360}s^3)$. An approximation to II order for all the series is sufficient to give all the terms in s^{-1} :

$$\mathcal{I}_0 = Res_{s=0} \left[e^{sx} \frac{\cosh\left(\frac{s m^*}{m}\right)}{s^2 \sinh s} \right] = a_{-1}$$

$$f(s) = \left(1 + sx + \frac{(sx)^2}{2!} + \dots\right) \left(1 + \frac{1}{2!} \left(s \frac{m^*}{m}\right)^2 + \dots\right) \frac{1}{s^2} \left(\frac{1}{s} - \frac{s}{6} + \dots\right)$$

We solve the products between parenthesis, and pick up just the terms in s^{-1} ,

$$Res_{s=0} = a_{-1} = \frac{1}{2} \left(x^2 - \frac{1}{3} + \left(\frac{m^*}{m} \right)^2 \right)$$

We will see that this three terms produce respectively the grand canonical potential in no field Ω_0 , the diamagnetic contribution, and the paramagnetic one, which we both put in Ω_{PL} .

2. Residues in $s = n\pi i$. We calculate the residues of the infinite simple poles in $s = n\pi i$, where the function diverges due to the denominator: $\sinh(ix) = \sin x$ and $\sin x = 0$ for every $x = n\pi$. This produces a series of real trms. Since the residue of $\sinh^{-1} s$ is 1 for $s = in\pi$, we get the series

$$\begin{aligned} \mathcal{I}(x) &= Res \sum_{n \neq 0} e^{in\pi x} \frac{\cosh(in\pi \frac{m^*}{m})}{(in\pi)^2 \sinh(in\pi)} \\ &= (-1) \sum_{n \neq 0} e^{in\pi x} \frac{\cos(n\pi \frac{m^*}{m})}{(n\pi)^2} Res\left(\frac{1}{\sin(n\pi)}\right) \\ &= -2 \sum_{n=1}^{\infty} \frac{\cos(n\pi x)}{(\pi n)^2} \cos(n\pi \frac{m^*}{m}) \end{aligned} \quad (59)$$

where we have converted the series on any integer n in a series only on the positive integers, noticing that:

$$\sum_{n \neq 0} e^{in\pi x} = \begin{cases} \cos(l\pi x) + i \sin(l\pi x) & n > 0 \\ \cos(l\pi x) - i \sin(l\pi x) & n < 0 \end{cases} = 2 \sum_{n=1}^{\infty} \cos(n\pi x)$$

where $l \in \mathbb{N}$ and we see that the imaginary part $i \sin$ cancels out for every n . If we consider the series in eq. (59), we see that, for Weierstrass criterion, it converges totally, and thus uniformly, since $|f(nx)| \rightarrow 0$ faster than $1/n$. This contribution to the potential Ω is responsible for the dHvA oscillations.

5.2 The grand canonical potential

$$\Omega = \Omega_0 + \Omega_{PL} + \Omega_{osc}$$

Pauli and Landau terms. We calculate $\Omega_0 + \Omega_{PL}$.

$$z(E) = \frac{A}{8\pi l^2} \hbar \omega_c \left(x^2 + \left(\frac{m^*}{m}\right)^2 - \frac{1}{3} \right)$$

we rewrite x , ω_c , A , to make it explicit the dependence on E , H :

$$z(E) = \frac{Am^*}{2\pi\hbar^2} E^2 + \frac{Am^*}{2\pi\hbar^2} \mu_B^2 \left(1 - \frac{1}{3} \left(\frac{m}{m^*}\right)^2 \right) H^2$$

We see that, besides the oscillating term, the grand canonical potential sums up to

$$\Omega - \Omega_{osc} = \int_0^\infty dE z(E) f'(E) = \underbrace{\frac{Am^*}{2\pi\hbar^2} \mu^2}_{\Omega_0} + \underbrace{\frac{Am^*}{2\pi\hbar^2} \mu_B^2 \left(1 - \frac{1}{3} \left(\frac{m}{m^*}\right)^2 \right) H^2}_{\Omega_{PL}} \quad (60)$$

where as in the 3D case, we have used the fact that for $\beta\mu \gg 1$ $f'(E) = -\delta(E - \mu)$. Since $M = -n\partial\Omega/\partial H$, where in 2D we define the particle density $n = N/A$, it is evident that the first term, which corresponds to the grand canonical potential of an inert gas, gives no contribution to the magnetization, as it is independent from H . For $m^* = m$ the Landau diamagnetic susceptibility is exactly $-1/3$ of Pauli's paramagnetic term.

The dHvA term. Here we evaluate Ω_{osc} . The exact derivative of the Fermi function is

$$f'(E) = -\frac{\beta}{4} \frac{1}{\cosh^2(\beta(E - \mu)/2)} \quad (61)$$

so that

$$\Omega_{osc} = \int_0^\infty dE z(E) f'(E) \quad (62)$$

$$= \frac{A}{8\pi l^2} \hbar \omega_c \beta \sum_{n=1}^{\infty} \frac{\cos(n\pi \frac{m^*}{m})}{(n\pi)^2} \underbrace{\int_0^\infty \frac{\cos(n\pi \frac{2E}{\hbar\omega_c})}{\cosh^2(\beta(E - \mu)/2)} dx}_{\otimes} \quad (63)$$

We consider now just \otimes , that is the relevant integral in E ; if we introduce the auxiliary variable $t = \frac{\beta}{2}(E - \mu)$ so that $dE = \frac{2}{\beta}dt$, the integral becomes

$$\otimes = \int_{-\mu\beta/2}^{\infty} dt \frac{\cos(n\pi \frac{4t}{\beta\hbar\omega_c} + n\pi 2\mu\hbar\omega_c)}{\cosh^2 t} \quad (64)$$

$$= \cos(n\pi \frac{2\mu}{\hbar\omega_c}) \int_{-\infty}^{\infty} dt \frac{\cos(\frac{4n\pi}{\beta\hbar\omega_c} t)}{\cosh^2 t} \quad (65)$$

The lower bound of the integral is taken to $-\infty$ in the condition $\mu\beta \gg 1$, and from the table of integrals (integral 3.982.1 GR [17])

$$\otimes = \frac{4n\pi^2}{\beta\hbar\omega_c} \cos(n\pi \frac{2\mu}{\hbar\omega_c}) \frac{1}{\sinh(\frac{2n\pi^2}{\beta\hbar\omega_c})} \quad (66)$$

The contribution of the simple poles on the imaginary axis reflects on the oscillating part of the grand canonical potential

$$\Omega_{osc} = \frac{A}{\pi\beta l^2} \sum_{n=1}^{\infty} \frac{1}{n} \frac{\cos(n\pi \frac{m^*}{m}) \cos(2n\pi \frac{\mu}{\hbar\omega_c})}{\sinh(\frac{2n\pi^2}{\beta\hbar\omega_c})} \quad (67)$$

we can see the oscillatory dependence (given by the cosine) on $1/\omega_c \approx 1/H$.

Another magnetic oscillatory effect is the *Shubnikov-de Haas effect*. It is an oscillation of magnetoresistance ρ_{ij} , detectable at low temperatures and in strong magnetic fields ($T \approx 1$ K, $H \approx 20$ T). As the dHvA effect, it arises from the quantization of the energy levels, and thus is another macroscopic effect of the intrinsic quantum nature of matter.

The interaction among electrons or the presence of impurities decreases the amplitude of dHvA oscillation, with a reduction factor known as the *Dingle factor*. In fact, if the electron scattering is taken into account, the Landau levels are broadened and this leads to a reduction in amplitude very nearly the same as would be caused by a rise of temperature from the real temperature T to $T + x$. The shift x is called the *Dingle temperature* and the Dingle factor is the amplitude reduction of oscillations given by $\exp(-2\pi^2 kx/\beta H)$ [1].

5.3 The Quantum Hall effect

1 - The integer quantum Hall effect. A spectacular effect of the quantization of the energy levels (LL) is the quantum Hall effect (QHE). The Hall voltage is quantized for a 2D system. In fact, we can view the dHvA effect as an outcome of the Quantum Hall effect; in turn, some consider the QHE a direct expression of gauge invariance in quantum systems. When a current \vec{J} passes through a conducting band in the presence of magnetic induction \vec{B} , a voltage V_H is produced in the direction normal to the current.

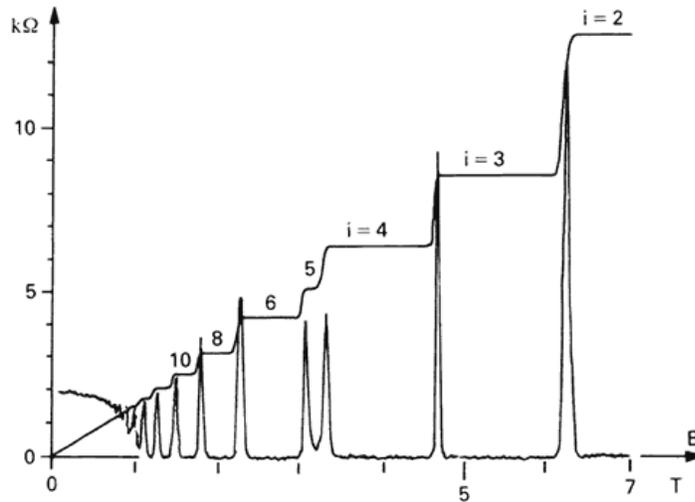


Figure 12: The Hall resistance varies stepwise with changes in magnetic field B . Step height is given by the physical constant $2\pi\hbar/e^2$ (value approximately 25 kilo-ohm) divided by an integer i . The figure shows steps for $i = 2, 3, 4, 5, 6, 8$ and 10. The lower peaked curve represents the longitudinal resistance, which disappears at each step; Yoshioka, [18]

2 - The fractional quantum Hall effect is a more complex phenomenon, which arises at lower temperatures and in stronger fields. It was explained with the introduction of *quasiparticles* by theoretical physicist Laughlin (for that, in 1998 he was awarded the Nobel prize). Quasiparticles are bound states of electrons and flux quanta of the field [19]. This field of research is very active and rapidly evolving and the theory it is concerned with goes

beyond the reaches of this short work - as it deals with the quantum theory of fields.

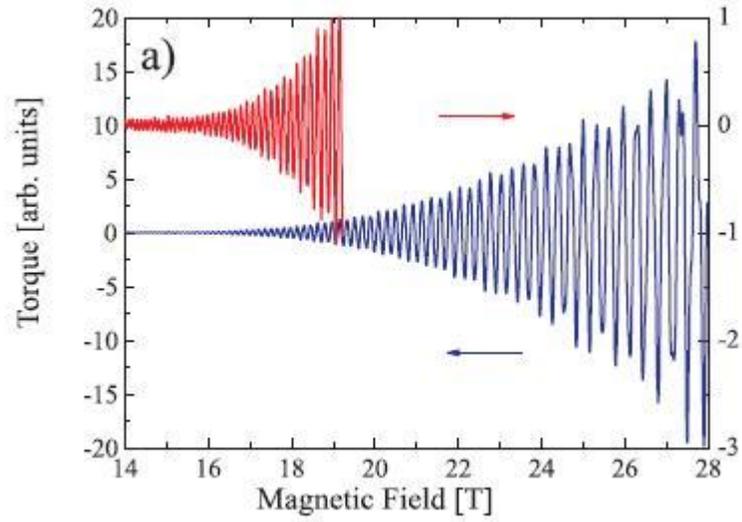


Figure 13: torque vs magnetic field. Gasparov, 2008 [8].

6 Conclusions

We have shown how to compute analytically the dHvA effect for noninteracting electrons in a magnetic field; the dHvA effect a subtle oscillatory behaviour of magnetization, not negligible in the regime $\mu_B H \gg k_B T$, which is of great interest in the study of superconducting properties of metals, since it is a reliable and precise tool to mapping the Fermi surface, which determines most of their electronic properties. We have explained the appearance of the Landau Levels, and given a basic quantum mechanical and statistical overview. We took inspiration from the paper of Sondheimer and Wilson [4] and show that also in 2D, magnetization is the sum of free concurrent terms: paramagnetism, diamagnetism and dHvA oscillations. We confuted the claim of Fujita *et al.*, 2002 [21], of the absence of diamagnetism in the 2DEG. We regard as an interesting feature the the fact that this is an exact derivation, through the means of Complex Analysis, of a calculation that is usually conducted through approximation methods (Euler-Maclaurin formula) [1, 21], or numerical implementation [7, 24]. We need to stress that this calculation is exact for the limiting case of noninteracting free electrons only, hence is open to wide approximation techniques as the knowledge of the crystal potential in metals is enhanced.

A comparison between the 3D and 2D cases shows that, introducing the identity $\mu = E_F$ for the Fermi gas at $T = 0$, the relevant physical quantities, Ω , M , χ are all expressed in terms of the density of states of the relative Fermi energy and D-dimensional volume. We use the relations for E_F and $\rho(E_F)$ in no magnetic field: In 3D:

$$E_F = \frac{\hbar^2}{2m^*} (3\pi^2 n)^{\frac{2}{3}} \quad \rho(E_F) = \frac{3N}{2V} E_F^{-1} = \frac{3n}{2E_F} \quad (68)$$

In 2D:

$$E_F = \frac{N\hbar^2}{Am^*} \quad \rho(E_F) = \frac{m^* A}{\pi\hbar^2} = \frac{2n}{E_F} \quad (69)$$

We can rewrite the magnetization and the susceptibility and see how they in

fact express the same physical relations in 3D and 2D:

$$\begin{aligned} M_{PL}(3D) &= \frac{4}{\sqrt{\pi}} V \mu_B^2 \sqrt{E_F} \left(\frac{m^*}{2\pi\hbar^2} \right)^{3/2} \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] H \\ &= V \mu_B^2 \rho(E_F) \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] H \end{aligned} \quad (70)$$

$$\begin{aligned} M_{PL}(2D) &= \frac{2N}{E_F} \mu_B^2 \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] H \\ &= A \rho(E_F) \mu_B^2 \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] H \end{aligned} \quad (71)$$

$$\chi_{PL}(3D) = \mu_B^2 \rho(E_F) \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] \quad (72)$$

$$\begin{aligned} \chi_{PL}(2D) &= \mu_B^2 \frac{2n}{E_F} \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] \\ &= \mu_B^2 \rho(E_F) \left[1 - \frac{1}{3} \left(\frac{m}{m^*} \right)^2 \right] \end{aligned} \quad (73)$$

We recall that the different term of the grand canonical potential Ω are:

$$\Omega = \Omega_0 + \Omega_{PL} + \Omega_{osc}$$

We report just the oscillatory part of Ω , responsible for the dHvA effect, both in the 3D and the 2D case:

$$\Omega_{osc}(3D) = \frac{V}{2\pi^2\beta} \left(\frac{eH}{4\hbar c} \right)^{3/2} \sum_{n=1}^{\infty} \frac{(-1)^n \cos\left(\frac{n\pi m^*}{m}\right) \cos\left(2n\pi \frac{\mu}{\hbar\omega_c} - \frac{\pi}{4}\right)}{(n)^{3/2} \sinh\left(\frac{2n\pi^2}{\beta\hbar\omega_c}\right)} \quad (74)$$

$$\Omega_{osc}(2D) = \frac{A}{\pi\beta} \frac{eH}{\hbar c} \sum_{n=1}^{\infty} \frac{1 \cos\left(n\pi \frac{m^*}{m}\right) \cos\left(2n\pi \frac{\mu}{\hbar\omega_c}\right)}{n \sinh\left(\frac{2n\pi^2}{\beta\hbar\omega_c}\right)} \quad (75)$$

We can recognize in both cases a dependence on the temperature and the magnetic field (from β and ω_c). The amplitude of the oscillations is modulated by $\cos(n\pi m^*/m)$. In both cases $\sinh^{-1} nx$ assures on the convergence of the series. We notice that, as reasonable, the series is multiplied by factors that have a difference in the exponents (3/2 in 3D, 1 = 2/2 in 2D), as the relevant D-dimensional volumes are V and A .

A Appendix

A.1 The Laplace transform

We define the Laplace transform of the function f

$$L[f] = \int_0^{\infty} e^{-sx} f(x) dx$$

provided that the infinite integral exists; s is a complex number. We notice that if $f(x) = 0$ for $x \leq 0$ the following relation holds

$$L[f](s) = F[f](is)$$

where $F[f]$ is the Fourier transform, $F[f] = \int_{-\infty}^{\infty} f(x)e^{i\omega x} dx$. In analogy with Fourier inversion theorem, it is possible to invert the Laplace transform,

$$f(x) = \frac{1}{2\pi i} \lim_{L \rightarrow \infty} \int_{s-iL}^{s+iL} F(\sigma) e^{\sigma x} d\sigma$$

where $s \geq s_1$ so that $F(\sigma)$ is analytic for $Re\sigma \geq s_1$, and the path is vertical. This formula is known as the Mellin inversion theorem. The function $f(x)$ is called the inverse Laplace transform of $F(s)$.

A.2 Peierls' method

A general proof of Peierls' method is given. We define

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

Proposition

$$\Omega = \int_0^{\infty} dE z(E) \phi''(E) \tag{76}$$

where

$$z(E) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{sE} \frac{Z_B(s)}{s^2},$$

s is the extension of β to the complex plane; $c \geq 0$ and

$$\phi(E) = -\frac{1}{\beta} \log(1 + e^{-\beta(E - \mu)})$$

is such that $\phi'(E) = f(E)$, where the latter is the Fermi function of eq.30.

Proof. We notice that the Laplace transform $\tilde{\phi}(s)$ is well defined for $Re(s) \geq -\beta$ and so is

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

Then we can evaluate Ω :

$$\begin{aligned} \Omega &= \sum_a g_a \phi(E_a) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{sE} \tilde{\phi}(s) \sum_a g_a e^{sE_a} \\ &= \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \tilde{\phi}(s) Z_B(-s) \\ &= \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} [\tilde{\phi}(s) s^2] \frac{Z_B(-s)}{s^2} \\ &= \int_0^\infty dE \phi''(E) z(E) \end{aligned}$$

To obtain the last line, the following relation for the resultant of the Laplace transform is used:

$$\int \frac{ds}{2\pi i} \tilde{f}(s) \tilde{g}(-s) e^{sx} = \int_0^\infty dy f(y) \int \frac{ds}{2\pi i} \tilde{g} e^{s(x-y)} = \int_{\max(x,0)}^\infty dy f(y) g(y-x)$$

A.3 The residue theorem

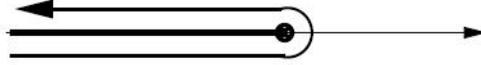
Consider a closed path γ , and a function f of complex variable z , that is holomorphic in the region enclosed by γ except for a collection, at most numerable, of isolated points (the *singularities*); the following applies:

$$\int_\gamma dz f(z) = 2\pi i \sum_n Res_{z_n}(f)$$

where z_n are all the singularities of f inside the contour γ . The residue of f is equal to the a_{-1} term of its Laurent series, defined as

$$f(z) = \sum_{-\infty}^{\infty} a_n z^n$$

Note that if f is completely holomorphic in the region considered, the Laurent series reduces to the Taylor series.

Figure 14: The path σ around the cut

A.4 Hankel's representation of the Γ function

The Gamma function is an extension to real and complex numbers of the factorial function $f(n) = n! = n \cdot (n-1) \cdot (n-2) \cdots 2 \cdot 1$, which is defined on positive integers; there are many representations of it. Euler, who first thought of it, devised the following integral representation

$$\Gamma(z) = \int_0^{\infty} dt e^{-t} t^{z-1} \quad (77)$$

defined for $\operatorname{Re}(z) > 0$; integrating by parts one obtains

$$\Gamma(z+1) = z\Gamma(z) \quad (78)$$

Its restriction to the positive integers is $\Gamma(n) = (n-1)!$. For $z = \frac{1}{2}$ the change $t = x^2$ makes eq. 77 equal to the Gaussian integral, so that $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. If we apply the functional relation eq.78 we can derive the relation

$$\Gamma(n + \frac{1}{2}) = \frac{(2n-1)!!}{2^n} \sqrt{\pi} \quad (79)$$

Hankel's integral representation of the Gamma function is

$$\frac{1}{\Gamma(z)} = \int_{\sigma} \frac{ds}{2\pi i} e^{s} s^{-z} \quad (80)$$

where σ is the path shown around the branch cut in figure 14.

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