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Landau diamagnetism and de Haas-van Alphen oscillations

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Chapter 1

Introduction

1.1 Summary

An electron can interact with a uniform magnetic field in 2 ways: through spin-field coupling and through orbit-field coupling. The first interaction is at the base of Pauli paramagnetism, discovered by Wolfgang Pauli in 1927, and the second interaction underlies Landau diamagnetism and de Haas-van Alphen effect, predicted and observed in 1930.

In this work we will concentrate on the consequences of this second coupling. In particular we will first analyse the case of a Bloch electron (electron in a lattice subject to a periodic potential) in a semiclassical context and we will obtain the quantization of the orbits' radius and energy. Moreover, we will deduce a periodicity in the structure of orbits to vary the field strength.

Then we will take into consideration the case of an almost free electron gas, which is a good approximation of the weakly bound electrons inside a metal. In this context it is possible to calculate analitically the magnetization, which happens to be composed of 2 factors: the first one linear in the field and the second one oscillating.

The frequencies of the oscillations for the Bloch electron and for the almost free electron gas are coherent and they are directly related to the geometry of the Fermi surface. The shape of the Fermi surface is involved in a lot of different phenomena (such as transport coefficients and optical characteristics) and the cited relation turns out to be a tool to measure it.

In particular, we now outline the major points of this work. First of all, we contextualise the canonical and grand canonical partition functions and free energies in the classical and quantum case for an electron gas assumed to be non interacting. In this treatment the classical Boltzmann single particle partition function

$$Z_1 = \int_{\Omega 1} \frac{d^3x d^3p}{h^3} e^{-\beta\epsilon(\vec{x},\vec{p})}$$

the quantum Boltzmann single particle partition function

$$Z_1 = \sum_{\alpha} g_\alpha e^{-\beta\epsilon_\alpha}$$

and the quantum grand canonical potential

$$\Omega = -\frac{1}{\beta}\sum_{\alpha} g_\alpha \ln\left(1 + e^{-\beta(\epsilon_\alpha - \mu)}\right)$$

have been used. The quantum grand canonical potential is directly connected with the average magnetization thanks to the relation $\langle M\rangle = -\frac{1}{V}\left.\frac{\partial\Omega}{\partial H}\right|_N$, hence to the magnetic susceptibility, which is defined as $\chi = \frac{\partial\langle M\rangle}{\partial H}$.

We start by analysing the response of a free electron gas in a classical framework, which leads to the absence of diamagnetism. This result is known as Bohr-van Leeuwen theorem and it proves that paramagnetism and diamagnetism must have a quantum origin.

Then we study the behaviour of a Bloch electron in a semiclassical framework and, using Bohr-Sommerfeld quantization of the action, we obtain an estimate of the fundamental frequency of de Haas-van Alphen oscillations in the magnetic susceptibility and its relation with the geometry of the Fermi surface

$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e}{\hbar c S_{ex}(\epsilon_F)}$$

where $S_{ex}(\epsilon_F)$ is the extremal cross section in k space of the Fermi surface evaluated at the Fermi energy.

At this point, we give an exact quantum treatment of an electron in a uniform magnetic field (Landau quantization and degeneracy of Landau levels) starting from the Hamiltonian

$$h = \frac{1}{2m^*}\left(\vec{p} + e\frac{\vec{A}(\vec{r})}{c}\right)^2 - \vec{\mu}\cdot\vec{H}$$

and obtaining the eigenvalue spectrum

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

with degeneracy at fixed k_z equal to $g = \frac{AeH}{2\pi\hbar c}$ and the eigenfunctions

$$\psi_{k_x k_z m_s n}(y) = \frac{1}{\sqrt{2^n n! l}\pi^{1/4}} e^{-\frac{(y-y_0)^2}{2l^2}} H_n\left(\frac{y-y_0}{l}\right) e^{i(k_x x + k_z z)}$$

Afterwards, we follow Landau's original derivation of the diamagnetic susceptibility of an electron gas in the case of low fields. He calculated the grand canonical potential by approximating the series

$$\Omega_{dia} = -\frac{eHV}{\beta 2\pi^2\hbar c}\sum_{n=0}^{\infty}\int_{-\infty}^{+\infty} dk_z \ln\left(1 + e^{-\beta\left(\frac{\hbar^2 k_z^2}{2m^*} + \hbar\omega_c\left(n+\frac{1}{2}\right) - \mu\right)}\right)$$

with an integral thanks to Euler-Maclaurin formula. This leads to

$$\chi_{dia} = -\frac{1}{3}\left(\frac{m}{m^*}\right)^2\frac{\mu_B^2}{V}\rho(\epsilon_F) = -\frac{1}{3}\left(\frac{m}{m^*}\right)^2\chi_{para}$$

which highlights the relation between the magnetic susceptibility due to the spin-field coupling (Pauli paramagnetism) and the one due to the orbit-field coupling (Landau diamagnetism).

In the end we obtain the magnetization and the magnetic susceptibility of a 2D and 3D electron gas by using Peierls' method. This exploits the relation between the grand canonical potential and the Boltzmann single particle partition function

$$\Omega = \int_0^{+\infty} d\epsilon \, \frac{df(\epsilon)}{d\epsilon} \mathscr{L}^{-1} \left[\frac{Z(s)}{s^2} \right] (\epsilon)$$

The calculation of the inverse Laplace transform requires an integral in the complex plane, done thanks to the residue theorem. It results that the grand canonical potential, hence also its derivatives (the magnetization and the magnetic susceptibility), is composed of 3 addends: Pauli paramagnetism, Landau diamagnetism and de Haas-van Alphen oscillations.

The first two addends are identical to the ones found by Landau, as long as we substitute the 2D or 3D density of states at the Fermi energy. The last addend, in the case of a 2D gas, is

$$\Omega_{osc} = \frac{AeH}{\pi \hbar c \beta} \sum_{n=1}^{+\infty} \frac{(-)^n}{n} \cos\left(n\pi \frac{m^*}{m} \right) \frac{\cos\left(\frac{2n\pi\mu}{\hbar\omega_c} \right)}{\sinh\left(\frac{2n\pi^2}{\beta\hbar\omega_c} \right)}$$

and in the case of a 3D gas becomes

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

This result is coherent with the semiclassical one obtained by Onsager, but less general, since it requires the electron gas to be almost free, which means that the Fermi surface is required to be almost spherical.

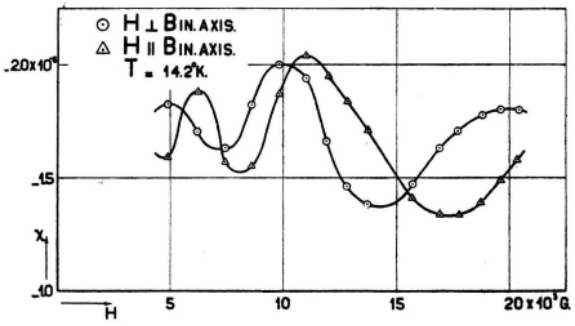

Figure 1.1: First observation of de Haas-van Alphen effect made by de Haas and van Alphen. We can see the experimental values of the magnetic susceptibility χ as a function of the external field H. *The dependence of the susceptibility of diamagnetic metals upon the field*, W. J. De Haas and P. M. Van Alphen, 1930.

1.2 History of the observations

W. J. de Haas was a physicist and a professor at Leiden university, Netherlands. In the late 1920s, he discovered, together with L. V. Shubnikov, the Shubnikov-de Haas effect, which is an oscillation in the conductivity of a material that occurs at low temperatures as a function of very intense magnetic fields. This was the inspiration that led De Haas and his student P. M. van Alphen in 1930 to measure the magnetization M of a sample of bismuth as a function of magnetic field in conditions of high fields at 14.2 K and to find oscillations in M/H (figure 1). The main technique exploited to measure the oscillations is based on the fact that in a field a magnetized sample experiences a torque proportional to its magnetic moment. This leads to the measure of the oscillations in angular postion of a sample of the metal, attached to a filar suspension, as the magnetic field strength varies.

Earlier that year, the 22-year-old Lev Landau, a Soviet physicist, was able to account for the oscillations in free electron theory, as a direct consequence of the quantization of closed electronic orbits in a magnetic field, and thus as a direct observational manifestation of a purely quantum phenomenon. He also pointed out a -1/3 ratio between the diamagnetic susceptibility he found and the already known paramagnetic susceptibility discovered by Pauli in 1927.

The theory for anisotropic system was put forward by Blackman in 1937 and compared with the experimental datas for the bismuth susceptibility (figure 2). In 1951, Sondheimer and Wilson were the first to evaluate the grand canonical potential for the electron gas immersed in a uniform magnetic field exploting Peierls' method, as it is done in this work.

The full extent of the usefulness of measuring the oscillations of the diamagnetic suscpetibility of the metals was only pointed out in 1952 by Onsager. He related the frequency of the oscillations to the shape of the Fermi surface, building a tool for its measurement. In 1952, Dingle explained that if collision broadening of the energy levels is taken into account, an extra damping factor must be included in equation (Dingle factor).

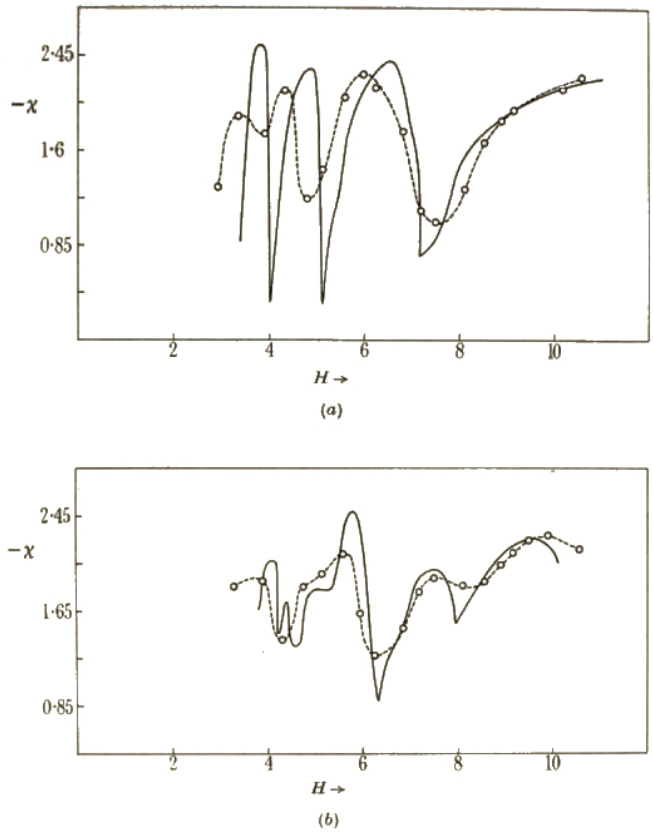

Figure 1.2: Blackman's comparison of the experimental $\chi - H$ curves with the theoretical curves for $T = 0$, (a) when the field is along the binary axis, (b) when the field is perpendicular to the binary axis. The experimental points are indicated in the curves. The susceptibility per unit volume is obtained by multiplying the ordinate by $9 \cdot 8 \times 10^{-6}$, the susceptibility per unit mass by multiplying by 10^{-6}. The unit for the abscissa is $10^3 G$. *On the diamagnetic susceptibility of bismuth*, M. Blackman, 1938.

1.3 The external magnetic field H

In this work we calculate the average magnetization per unit volume, which will be derived thanks to the relation $\langle M \rangle = -\frac{1}{V} \frac{\partial F}{\partial H}\big|_N$. F represents the canonical free energy (it can be replaced with the grand canonical free energy Ω), which will be defined in the next chapter. The magnetic susceptibility is defined as $\chi := \frac{\partial \vec{M}}{\partial H}$, where H is the external magnetic field, which is related to B through the equation $B = H + 4\pi M$.

Since in an experiment we have control on H and $4\pi M$ is a negligible correction in comparison with H, we calculate M taking the derivative with respect to H and substituting H in place of B everywhere in the following derivations.

Chapter 2

Statistical mechanics

2.1 Classical statistical mechanics

From a classical point of view, our system is a gas composed of point particles with electric charge $-e$. We define the *canonical partition function* of the system

$$Z := \int_{\Omega} \frac{d^{3N}x d^{3N}p}{N! h^{3N}} e^{-\beta E} \tag{2.1}$$

where E is the total energy of the gas and the $N!$ factor is due to the fact that interchanging the coordinates of two electrons gives rise to a classically equivalent configuration of the system. The integral is taken over the phase space volume Ω of allowed configurations of the system and the presence of the Planck constant is just an arbitrary normalization.

The considered system is an ideal gas in the sense that we assumed the electrons to be non interacting, and thanks to this hypothesis we can write the total energy of the gas as $E = \sum_{i=1}^{N} \epsilon(\vec{x}_i, \vec{p}_i)$, where $\epsilon(\vec{x}_i, \vec{p}_i)$ is the single particle energy, function of the 6 coordinates $\vec{x}_i$ and $\vec{p}_i$ in the phase space.

Therefore the partition function can be factored as $Z = \frac{1}{N!} \prod_{i=1}^{N} Z_i = \frac{1}{N!} Z_1^N$, where

$$Z_1 = \int_{\Omega 1} \frac{d^3x d^3p}{h^3} e^{-\beta \epsilon(\vec{x}, \vec{p})} \tag{2.2}$$

since the energy of each electron ϵ is the same function of the coordinates $\vec{x}_i$ and $\vec{p}_i$. The canonical partition function Z contains all the information about the system and it can be used to calculate the *canonical free energy*

$$F := -\frac{1}{\beta} \ln(Z) \tag{2.3}$$

which for a non interacting gas becomes

$$F = -\frac{N}{\beta} \ln\left(\frac{Z_1}{N!}\right) \tag{2.4}$$

The average magnetization, which we are interested in, is defined in the canonical ensemble as $< M >= -\frac{\partial F}{\partial H}$.

2.2 Quantum statistical mechanics

Electrons are fermions with $s = 1/2$. In our system we have a certain number of electrons confined inside a box. The global wave function of all electrons, since they have semi-integer spin, must be antisymmetric under interchange of any 2 electrons. Pauli exclusion principle is a direct consequence of this global wave function characteristic and it states that 2 identical fermions (in our case electrons) can never occupy the same quantum state, otherwise the global wave function would be symmetric under their interchange. This fact plays a very important role in the behaviour of an electron gas, expecially at low temperature, which is our case.

In our analysis the electrons are assumed to be non interacting, therefore the global Hamiltonian $\mathcal{H}$ can be decomposed as the sum of the N single electron Hamiltonians h

$$\mathcal{H} = \sum_{j=1}^{N} h(\vec{p_j}, \vec{r_j}, \vec{\sigma}_j) \tag{2.5}$$

where $\vec{p}_j$, $\vec{r}_j$ and $\vec{\sigma}_j$ are respectively the momentum, position and spin operators of the j-th electron. The operators relative to different electrons commute, hence the single particle Hamiltonians $[h(\vec{p}_i, \vec{r}_i, \vec{\sigma}_i), h(\vec{p}_j, \vec{r}_j, \vec{\sigma}_j)] = 0$ So, in general, the single electron wave function is a solution of the equation $h\psi_k = \epsilon_k \psi_k$, with ϵ_k eigenvalue of the k-th eigenstate of the single electron Hamiltonian. Now the wave function of a generic state of the system is built antisymmetrising the considered single particle eigenfunctions (Slater determinant) as follows

$$\Psi(\vec{r}_1, \vec{\sigma}_1, ..., \vec{r}_N, \vec{\sigma}_N) = \frac{1}{\sqrt{N!}} \sum_P (-)^P \prod_k \psi_k(\vec{r}_{P(1)}, \vec{\sigma}_{P(1)}, ..., \vec{r}_{P(N)}, \vec{\sigma}_{P(N)}) \tag{2.6}$$

where the sum is taken over all possible permutations P of the electron index and the product is taken over the k single particle eigenstates considered.

$\Psi_{\bar{k}}$ is the $\bar{k}$-th solution of the Schrödinger equation $\mathcal{H}\Psi_{\bar{k}} = E_{\bar{k}}\Psi_{\bar{k}}$ and using the relations (2.5) and (2.6), we obtain $E = \sum_k \epsilon_k$ which means that the energy of the state of a set of non interacting electrons is the sum of the energies of the states that have been antisymmetrised to build it.

Now we analyse in a quantum context the already mentioned single particle canonical partition function particle (2.2)

$$Z_1 := tr\left(e^{-\beta h}\right) = \sum_k e^{-\beta \epsilon_k} = \sum_\alpha g_\alpha e^{-\beta \epsilon_\alpha} \tag{2.7}$$

where the trace is taken over all possible eigenfunction ψ_k of the operator h. This is equivalent to summing over all possible ϵ_α eingenvalues of h taking into account the degeneracy of each eigenvalue g_α.

We also introduce the *grand canonical partition function* Ξ of the system, which is defined as

$$\Xi := tr\left(e^{-\beta(\mathcal{H} - \mu N)}\right) \tag{2.8}$$

where N intended as an operator and μ is called the *chemical potential*. Now we elaborate the formula in our conditions

$$\Xi = \sum_{N=0}^{\infty} \sum_{\bar{k}} e^{-\beta\left(\sum_k \epsilon_k - \mu N\right)} =$$

where the first sum is taken over all possible N numbers of electrons and the second sum is taken over all possible $\bar{k}$ eigenstates of the system's Hamiltonian $\mathcal{H}$. This is equivalent to the summation

$$= \sum_{N=0}^{\infty} \sum_{n_k} e^{-\beta \sum_k (\epsilon_k - \mu) n_k} = \sum_{N=0}^{\infty} \sum_{n_k} \prod_k e^{-\beta(\epsilon_k - \mu) n_k} =$$

where n_k is the number of electrons occupying the k-th eigenstate with the restriction $\sum_k n_k = N$. Extending the second summation over all possible n_k, we can remove the last condition and the summation over all possible N. Therefore

$$= \sum_{n_k} \prod_k e^{-\beta(\epsilon_k - \mu) n_k} = \prod_k \sum_n e^{-\beta(\epsilon_k - \mu) n} = \prod_k \left(1 + e^{-\beta(\epsilon_k - \mu)}\right)$$

since two fermions can never occupy the same quantum state, so the only possibilities are $n = 0, 1$

$$\Xi = \prod_k \left(1 + e^{-\beta(\epsilon_k - \mu)}\right) \tag{2.9}$$

The last quantity we introduce is the *grand canonical potential* (grand canonical free energy), which is defined as

$$\Omega := -\frac{1}{\beta} \ln \Xi \tag{2.10}$$

and thanks to equation (2.9) we can write in our context

$$\Omega = -\frac{1}{\beta} \sum_k \ln\left(1 + e^{-\beta(\epsilon_k - \mu)}\right) = -\frac{1}{\beta} \sum_\alpha g_\alpha \ln\left(1 + e^{-\beta(\epsilon_\alpha - \mu)}\right) \tag{2.11}$$

From the grand canonical potential, the average magnetization, which we are interested in, is defined in the grand canonical ensemble as $< \vec{M} >:= -\frac{1}{V}\frac{\partial \Omega}{\partial H}$ and similarly the average number of electrons $< \vec{N} >:= -\frac{\partial \Omega}{\partial \mu}$.

Chapter 3

Classical treatment

Bohr-van Leeuwen theorem states that diamagnetism can not occur in a classical system at the equilibrium. First we give a non-formal insight on the 2D phenomenon.

We consider N electrons confined inside a 2D large circular box of radius R as in figure 3.1. The collisions of the electrons with the edge of the box are assumed to be elastic. The area of the box is $A = \pi R^2$ and the density of the electrons $n = \frac{N}{A}$ is uniform inside the box. The electrons are immersed in a magnetic field orthogonal to the 2D box, therefore each electron is subject to the Lorentz force $\vec{F} = -\frac{e}{c}\vec{v} \times \vec{H}$, which is a centripetal force since it is by definition orthogonal to the velocity. We obtain the relation for the magnitude $\frac{mv^2}{r} = \frac{e}{c}vH$. This causes the trajectories to be circumferences of radius $r = \frac{v}{\omega_c}$, where $\omega_c := \frac{eH}{mc}$ is the cyclotron frequency, all run in the same direction.

The magnetic moment of each electron can be calculated as $\mu = -\frac{e\vec{L}}{2m}$ where $\vec{L} = \vec{\rho} \times m\vec{v}$ is the angular momentum of the considered electron with respect to an origin common to every electron. We choose the common origin to be, for instance, the point B in figure 3.1. When electron 2 passes through the small element enclosed by the square, it has the same angular momentum of electron 1 when it passes through this element, but with opposite direction. Since electrons are uniformly distributed in the box, it is clear that for each electron passing through a given point in the box with a certain velocity, there is another electron passing through the same point with the same velocity but with opposite direction. The electrons near the boundary, like electron 1, collide with the edge and bounce elastically along the edge, forming a sequence of arcs of circumference. These electrons play a fundamental role in the absence of diamagnetism in classical models because, without them, electrons passing near the edge can not be compensated.

Now we exhibit a formal proof. We consider N electrons as a 3D classical ideal (non interacting) gas of charged particles in a volume V. The magnetization $\vec{M}$ of the gas is the total magnetic moment of the electrons per unit volume.

The total Hamiltonian of the system, in the case of an electron gas, it can be written in the form

$$\mathcal{H} = \frac{1}{2m}\sum_{i=1}^{N}\left(\vec{p}_i + \frac{e\vec{A}(\vec{r}_i)}{c}\right)^2 \tag{3.1}$$

where $\vec{p}_i$ is the generalised momentum of the i-th electron and $\vec{A}$ is the vector

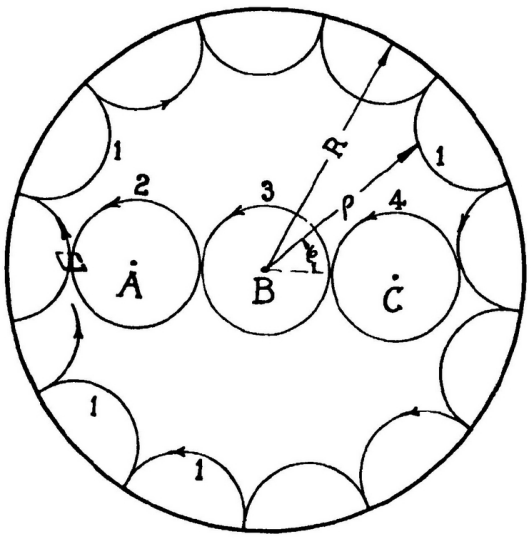

Figure 3.1: A representation of the behaviour of classical charged particles confined in a circular 2D box with elastic edge. *The theory of electric and magnetic susceptibilities*, J. H. van Vleck, 1932.

potential of the field $\vec{H}$. In the canonical ensemble formalism, we calculate the average value of the magnetization as $< \vec{M} >= -\frac{1}{V}\frac{\partial F}{\partial H}$ and from equation (2.4) we write

$$F = -\frac{N}{\beta} \ln \left(\int_V \frac{d^3x}{N!h^3} \int_{-\infty}^{+\infty} d^3p \, e^{-\frac{\beta}{2m}\left(\vec{p}+\frac{e\vec{A}(\vec{r})}{c}\right)^2} \right)$$

Defining the mechanical momentum $\vec{\Pi}_i = p_i + \frac{e}{c}\vec{A}$ of the i-th electron and substituting it makes the integrand independent on the field $\vec{H}$ and does not affect the ends of the integral (since they are $\pm\infty$). Therefore the derivative of F with respect to H must vanish and no magnetization can occur.

Chapter 4

Onsager semiclassical treatment

4.1 Semiclassical motion

A semiclassical treatment has been provided by Onsager using Bohr-Sommerfeld quantization. This consists, first, in deriving the motion of an electron inside a lattice (*Bloch electron*) immersed in a magnetic field $\vec{H}$ from the known Hamilton's equations of motion.

Denoting by $\vec{k}$ the generalised wave vector of the electron and by $\vec{A}(\vec{r})$ the vector potential of the magnetic field, we define the mechanical wave vector of the electron as

$$\vec{K} := \vec{k} + \frac{e}{\hbar c}\vec{A}(\vec{r}) \tag{4.1}$$

The equations of motion are

$$\hbar\frac{dk_i}{dt} = -\frac{\partial h}{\partial r_i} \tag{4.2}$$

$$v_i = \frac{\partial h}{\hbar \partial k_i} \tag{4.3}$$

where h is the single particle Hamiltonian and i stands for the i-th component of the vectors. Keeping in mind the aim of taking into account the presence of the lattice (that is a periodic potential), we make the general assumption of a single electron Hamiltonian of the form $h = \epsilon\left(\vec{k} + \frac{e}{\hbar c}\vec{A}(\vec{r})\right) = \epsilon(\vec{K})$.

Introducing the wave vector $\vec{K}$ in equation (4.2) we can write

$$\hbar\frac{dK_i}{dt} - \frac{e}{c}\frac{dA_i(\vec{r})}{dt} = -\frac{\partial h}{\partial r_i} = -\frac{\partial K_j}{\partial r_i}\frac{\partial h}{\partial K_j} \tag{4.4}$$

and in equation (4.3)

$$\hbar v_i = \frac{\partial K_j}{\partial k_i}\frac{\partial h}{\partial K_j} = \frac{\partial h}{\partial K_i} \tag{4.5}$$

Considering the last term in equation (4.4), we calculate the first factor and we recognise in the second factor equation (4.5), obtaining

$$\hbar\frac{dK_i}{dt} = -\frac{e}{\hbar c}\frac{\partial A_j(\vec{r})}{\partial r_i}\hbar v_j + \frac{e}{c}\frac{dA_i(\vec{r})}{dt} = -\frac{e}{c}\left(v_j\frac{\partial A_j(\vec{r})}{\partial r_i} - v_j\frac{\partial A_i(\vec{r})}{\partial r_j}\right)$$

In the last term of the above expression we can recognise $\left(\vec{v} \times (\vec{\nabla} \times \vec{A})\right)_i$, and in the end the equations of motion become

$$\hbar v_i = \frac{\partial \epsilon}{\partial K_i} \tag{4.6}$$

$$\hbar \frac{dK_i}{dt} = -\frac{e}{c}(\vec{v} \times \vec{H})_i \tag{4.7}$$

where we have used the relation $\vec{H} = \vec{\nabla} \times \vec{A}$.

Since $\vec{H}$ is uniform, without loss of generality we assume it in the z direction $\vec{H} = (0, 0, H)$. The first equation of motion (4.6) can be written in the form

$$\frac{d}{dt}\left(\hbar \vec{K} + \frac{e}{c}\vec{r} \times \vec{H}\right) = 0$$

since $\vec{H}$ does not vary with time. Solving and projecting the above equation in the $K_x - K_y$ plane leads to

$$\vec{K}_\perp = -\frac{e}{\hbar c}(\vec{r}_\perp - \vec{r}_{0\perp}) \times \vec{H} \tag{4.8}$$

At fixed ϵ and K_z, calling $\vec{\mathcal{A}}(\epsilon, K_z)$ the area of the orbit of the electron in the $x-y$ plane and $\vec{S}(\epsilon, K_z)$ the area of the orbit of the electron in the $K_x - K_y$ plane, we now prove that

$$\vec{S}(\epsilon, K_z) = \left(\frac{eH}{\hbar c}\right)^2 \vec{\mathcal{A}}(\epsilon, K_z) \tag{4.9}$$

Differentiating equation (4.8) we obtain

$$d\vec{K}_\perp = -\frac{e}{\hbar c}(d\vec{r}_\perp \times \vec{H})$$

and, thanks to this, we can write

$$\vec{S}(\epsilon, K_z) = \frac{1}{2}\oint \vec{K}_\perp \times d\vec{K}_\perp = \left(\frac{e}{\hbar c}\right)^2 \frac{1}{2}\oint (\vec{r}_\perp \times \vec{H}) \times (d\vec{r}_\perp \times \vec{H}) =$$

which, using the properties of the vector product, becomes

$$= \left(\frac{eH}{\hbar c}\right)^2 \frac{1}{2}\oint \vec{r}_\perp \times d\vec{r}_\perp = \left(\frac{eH}{\hbar c}\right)^2 \vec{\mathcal{A}}(\epsilon, K_z)$$

4.2 Bohr-Sommerfeld quantization

Bohr-Sommerfeld relation for the quantization of the action is

$$\left|\oint_{\gamma_n} \vec{k} \cdot \vec{dl}\right| = 2\pi\left(n + \frac{1}{2}\right) \tag{4.10}$$

where the integral is taken along the n-th electron orbit γ_n and the addend $\frac{1}{2}$ is a correction made for the system under consideration.

Substituting the definition of the generalised wave vector (4.1), we obtain

$$\left| \oint_{\gamma_n} \vec{K} \cdot \vec{dl} - \frac{e}{\hbar c} \oint_{\gamma_n} \vec{A} \cdot \vec{dl} \right| = 2\pi \left(n + \frac{1}{2} \right)$$

We can replace $\vec{K}$ with this expression in the first integral and, thanks to Stokes' theorem, we can write

$$\left| -\frac{e}{hc} \oint_{\gamma_n} \left[(\vec{r} - \vec{r}_0) \times \vec{H} \right] \cdot \vec{dr} - \frac{e}{hc} \int_{\mathcal{A}_n} (\nabla \times \vec{A}) \cdot d\vec{\mathcal{A}} \right| = n + \frac{1}{2}$$

where $\mathcal{A}_n$ is the area within the orbit γ_n.

The integral along the closed path γ_n of $\vec{r}_0 \times \vec{H}$ vanishes since it is a constant vector and by definition $\vec{H} = \nabla \times A$, so calling Φ the flux of the magnetic field $\vec{H}$ across S it results

$$\left| -\frac{e}{hc} \oint_{\gamma_n} (\vec{r} \times \vec{H}) \cdot \vec{dr} - \frac{e}{hc} \Phi \right| = n + \frac{1}{2}$$

Using the triple product relation, the formula $\oint_{\gamma_n} \frac{1}{2} \vec{r} \times \vec{dr} = \vec{\mathcal{A}}_n$ and defining $\Phi_0 := \frac{eh}{c}$, in the end the equation becomes $\Phi = \left(n + \frac{1}{2} \right) \Phi_0$.

The flux quantization impose a minimal circular orbit dimension $\Phi_0 = H\pi l^2$ which have radius $l = \sqrt{\frac{\hbar c}{eH}}$, also called *magnetic length*, and the more energetic orbits have quantized radius $R_n = l\sqrt{n + \frac{1}{2}}$.

4.3 Onsager derivation of the de Haas-van Alphen oscillations frequency

In addition, we can elaborate differently the semiclassical condition for the quantization (4.10), in order to obtain an estimate for the frequency of the de Haas-van Alphen oscillations.

Although it may seem unnatural in a system with cylindrical symmetry not to choose a symmetric vector potential $\vec{A}$ in the $x \Leftrightarrow y$ interchange, the following is the easiest way of derivation. The choice $\vec{A} = (-Hy, 0, 0)$ is called the *Landau gauge* and it leads to the correct magnetic field $\vec{H} = \nabla \times \vec{A}$.

We can write the components of the relation (4.1) in the form

$$\begin{cases} K_x = k_x - \frac{eHy}{\hbar c} \\ K_y = k_y \\ K_z = k_z \end{cases}$$

hence the quantization condition as follows

$$\left| \oint_{\gamma_n} k_x dx + \oint_{\gamma_n} k_y dy \right| = 2\pi \left(n + \frac{1}{2} \right)$$

Since we have chosen the vector potential $\vec{A}$ only dependent on y coordinate, the motion of the electron in the x direction remains the same as in the lattice without the magnetic field. Therefore k_x is constant and its integral along a closed path vanishes.

Differentiating the first relation of the system $dK_x = -\frac{eH}{\hbar c}dy$ we can write

$$S_n(\epsilon, k_z) = \oint_{\gamma_n} K_y dK_x = \frac{2\pi eH}{\hbar c}\left(n + \frac{1}{2}\right) = \Delta S(\epsilon, k_z)\left(n + \frac{1}{2}\right) \tag{4.11}$$

where we have recognised in the first term the area $S_n(\epsilon, k_z)$ of the circle in the k-space at fixed k_z and energy up to ϵ and $\Delta S(\epsilon, k_z)$ the difference between the areas of two succeeding levels. Equation (4.11) is known as *Onsager relation* and it is directly connected to the flux quantization $\Phi = \left(n + \frac{1}{2}\right)\Phi_0$ through equation (4.9).

At fixed k_z we can approximate the quantity

$$(\epsilon_{n+1} - \epsilon_n)\frac{S_{n+1}(\epsilon_{n+1}, k_z) - S_n(\epsilon_n, k_z)}{\epsilon_{n+1} - \epsilon_n} = \frac{2\pi eH}{\hbar c}$$

in the limit $n \gg 1$ (equivalent to the limit H weak field) with

$$(\epsilon_{n+1} - \epsilon_n)\frac{\partial S(\epsilon, k_z)}{\partial \epsilon} = \frac{2\pi eH}{\hbar c}$$

Classically the *cyclotron frequency* is defined as $\omega_c := \frac{eH}{mc}$. In our context we can generalise this definition at costant k_z in the form $\hbar\omega_c = \epsilon_{n+1} - \epsilon_n$, and this leads to a natural definition of the effective mass of the electron

$$m^* = \frac{\hbar^2}{2\pi}\left(\frac{\partial S(\epsilon, k_z)}{\partial \epsilon}\right)^{-1} \tag{4.12}$$

We can notice that, for an increase in H such that $S_{n+1}(\epsilon, k_z) = S_n(\epsilon, k_z) = S(\epsilon, k_z)$, the electron orbit are the same as before the increase, hence the magnetic properties in which we are interested. We obtain the conditions

$$\frac{S(\epsilon, k_z)}{H_n} = \frac{2\pi e}{\hbar c}\left(n + \frac{1}{2}\right) \quad \frac{S(\epsilon, k_z)}{H_{n+1}} = \frac{2\pi e}{\hbar c}\left(n + \frac{3}{2}\right)$$

and in the end the relation

$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e}{\hbar c S(\epsilon, k_z)}$$

From the formula, it appears evident that the period is dependent on the k_z value, therefore we would expect an almost continuous period spectrum. However, it can be shown that the main contributions to the magnetization at fixed ϵ are due to the k_z values such that S is extremal (maximum or minimum), that is $\frac{\partial S(\epsilon, k_z)}{\partial k_z}\Big|_{k_{zex}} = 0$ and $S_{ex}(\epsilon) = S(\epsilon, k_{zex}(\epsilon))$. Since $S_{ex}(\epsilon)$ is in general a growing function of the energy, the fundamental period (the shortest) is

$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e}{\hbar c S_{ex}(\epsilon_F)} \tag{4.13}$$

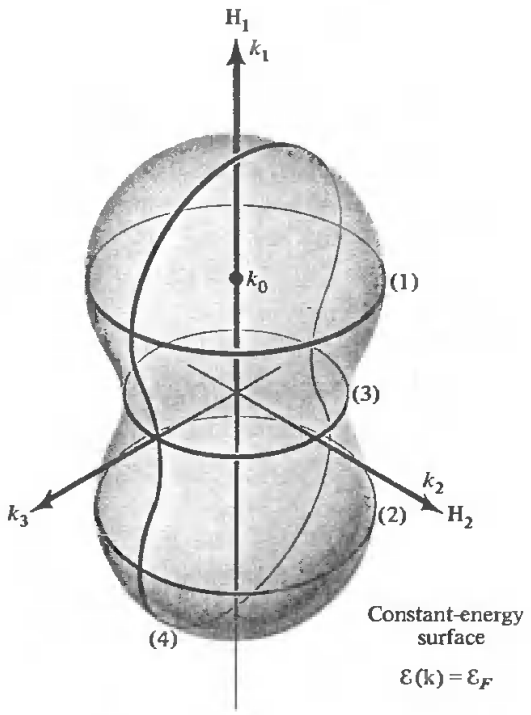

Figure 4.1: Extremal surfaces of a general shape of the Fermi surface, with repsect to different directions of the magnetic field.

4.4 Tomography of the Fermi surface

The equation (4.13) shows that the de Haas-van Alphen phenomenon can be used as a tool for the *tomography* of the Fermi surface of a metal. In fact, the measurement of the area of the extremal surfaces in k-space orthogonal to the field leads to a complete map of the Fermi surface. This is carried out by measuring the period of the oscillations as a function of the field direction. The importance of the knowledge of the Fermi surface is that it is involved in the derivation of a lot of properties of the material, such as the transport coefficients and optical characteristics.

Chapter 5

Quantum treatment

5.1 Landau levels

We start now with an exact quantum approach of the motion of an electron immersed in a magnetic field.

We will take into consideration the presence of the lattice allowing the possibility for an effective mass m^*, as already done above. For a matter of simplicity in the following derivations we will exclude the possibility for m^* to be dependent from E, from k_z, or from the direction of the magnetic field. In practice, this means that m^* will replace m in every kinetic term, but obviously not in the interaction between the intrinsic magnetic moment of the electrons and the magnetic field. This is accurate only for the electrons in the metal which are very weakly bound to atoms' nuclei and which are near the bottom of a symmetric band, where the energy may be assumed proportional to k^2, and where the Fermi surface is almost spherical.

The general Hamiltonian of such a system is

$$h = \frac{1}{2m^*}\left(\vec{p} + e\frac{\vec{A}(\vec{r})}{c}\right)^2 - \vec{\mu}\cdot\vec{H} \tag{5.1}$$

and introducing the conditions $\vec{H} = (0, 0, H)$ of uniform field and $\vec{\mu} = -2\mu_B\frac{\vec{S}}{\hbar}$ for the electron, we obtain

$$h = \frac{p^2}{2m^*} - \frac{e}{m^*}\left(2\vec{A}\cdot\vec{p} + \left[\vec{p}, \vec{A}\right]\right) + \frac{e^2A^2}{2m^*c^2} + 2\frac{\mu_B}{\hbar}S_zH$$

As already done above, we impose the Landau gauge $\vec{A} = (-Hy, 0, 0)$. Thanks to the relation $\left[\vec{p}, \vec{A}\right] = -i\hbar\nabla\cdot\vec{A} = 0$, the Hamiltonian becomes

$$h = \frac{1}{2m^*}\left[\left(p_x - eH\frac{y}{c}\right)^2 + p_y^2 + p_z^2\right] + 2\frac{\mu_B}{\hbar}S_zH$$

It follows that h, p_x, p_z and S_z are a complete set of commuting observables, the eigenfunctions can be labelled with the quantum numbers k_x, k_z (whose allowed values are all the real numbers) and $m_s = \pm 1$ and they can be written in the form $\psi_{k_xk_zm_s} = e^{i(k_xx+k_zz)}\chi_{m_s}(y)$.

Substituting this expression in the Schrödinger equation $h\psi = \epsilon\psi$ together with the quantities $y_0 = \frac{\hbar c k_x}{eH}$ centre of the armonic oscillator and $\omega_c = \frac{eH}{m^* c}$ cyclotron frequency and simplifying the plane wave component, the result is

$$-\frac{\hbar^2}{2m^*}\chi''_{m_s} + \frac{m^*\omega_c^2}{2}(y-y_0)^2\chi_{m_s} = \left(\epsilon - \frac{\hbar^2 k_z^2}{2m^*} - m_s\mu_B H\right)\chi_{m_s} \tag{5.2}$$

This is the equation for a monodimensional harmonic oscillator centred in y_0, with angular frequency ω_c. Then, it is known that the energy eigenvalues are

$$\epsilon_{k_z m_s n} = \hbar\omega_c(n+\frac{1}{2}) + \frac{\hbar^2 k_z^2}{2m^*} + m_s\mu_B H \tag{5.3}$$

for $n = 0, 1, 2, ...$ and the eigenfunctions are

$$\chi_{k_x k_z m_s n}(y) = \frac{1}{\sqrt{2^n n! l}\pi^{1/4}} e^{-\frac{(y-y_0)^2}{2l^2}} H_n\left(\frac{y-y_0}{l}\right) \tag{5.4}$$

where H_n is the n-th Hermite polinomial and l is the already defined magnetic length. l can be thought as a measure of the localization of the electron, and in the mentioned experiments, for a magnetic field of $10^3 G$ and an electron of $2eV$ of energy, it is approximately $l_t \approx 5 \cdot 10^{-3} cm$.

For what has been said so far, in the Hamiltonian spectrum there are three components: Landau levels (descrete and due to the armonic oscillator), spin-field coupling (descrete) and kinetic energy (continuous and due to the free motion in the z direction). Since its eigenvalues do not depend on k_x, they are infinitely many times degenerate.

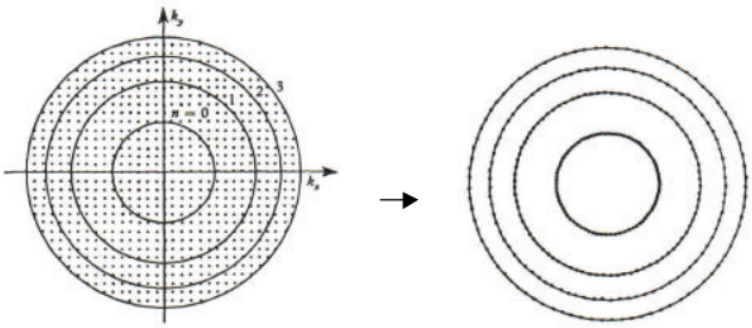

Figure 5.1: States' rearrangement of the electrons of a free gas when immersed in a magnetic field.

5.2 Degeneracy of Landau levels

The next condition that has to be applied to the electron is the confinement in a box of dimensions $L \times L \times L$.

First we consider an electron with fixed k_z value and we assume an infinite potential outside the 2D region of coordinates $[0, L] \times [0, L]$. This implies that the wave function has to vanish on the boundary $\psi(0, y, z) = \psi(L, y, z) = \psi(x, 0, z) = \psi(x, L, 0) = 0$, hence $k_x = \frac{2\pi n_x}{L}$ and $k_y = \frac{2\pi n_y}{L}$ for $n_x, n_y \in \mathbb{Z}$.

The eigenfunctions ψ for which the centre y_0 lies well inside the volume will not be affected by the presence of the walls. No solutions exist if y_0 lies well outside the volume and for a small range of y_0 near the wall, the presence of the wall modifies the oscillator eigenfunction and raises the energy value. This can be justified by the Heinsberg uncertainty principle $\Delta x \Delta p \geq \frac{\hbar}{2}$ since, as the centre y_0 gets closer to the boundary, the electron is subject to the overlap of the armonic potential and of the increasingly dominant wall potential. This implies that the electron is more and more localised, therefore its momentum has to rise, hence its energy. In the following discussion we will neglect the border region effect and we will impose the condition for the centre of the armonic oscillator $0 < y_0 < L$. This approximation is valid assuming that $L >> l_t$.

Substituting the definition of y_0 we obtain $0 < n_x < \frac{L^2 eH}{2\pi\hbar c}$. So the number of allowed n_x values is exactly $g = \frac{L^2 eH}{2\pi\hbar c}$, which is the *degeneracy* of each Landau level at fixed k_z. In the last relation we can recognise the flux $\Phi = L^2 H$ of the magnetic field and the quantum of flux $\Phi_0 = \frac{2\pi\hbar c}{e}$. The degeneracy, that is the number of states available for the electron, can be rewritten in the form of the number of flux quanta Φ_0 flowing through the cross-section.

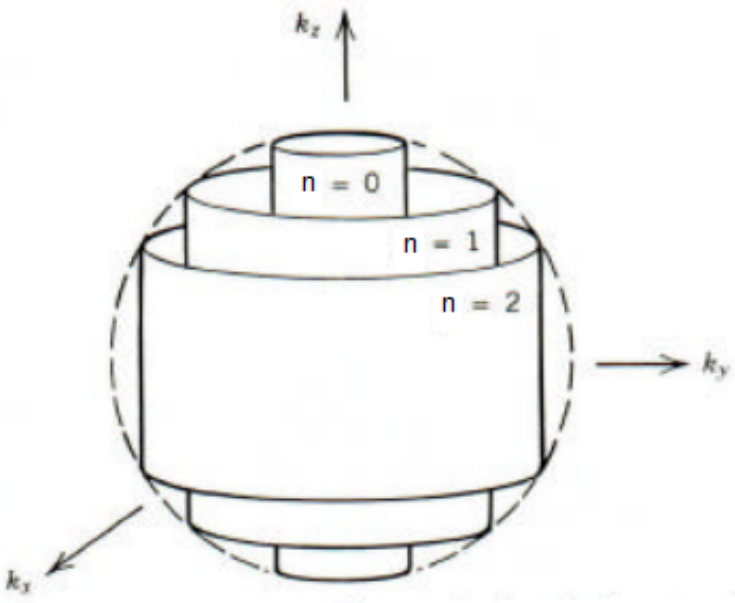

Figure 5.2: Fermi surface of a free electron gas immersed in a uniform magnetic field, also known as Landau tubes.

Another way of deriving this result is to start from the electron in the box without any magnetic field. The available states (points in the $\vec{k}$ space) form a 3D equally $\frac{2\pi}{L}$ spaced grid inside the Fermi sphere. Fixing k_z leaves us with 2D grid inside a circle in the $k_x - k_y$ plane (left image in figure 5.1). The squared radius (in k-space) is $R^2 = \epsilon_F - \frac{\hbar^2 k_z^2}{2m^*}$.

Introducing the magnetic field causes a rearrangement of these states in a different configuration. Landau levels can be viewed as concentric circumferences of squared radius $R^2 = \frac{2m^*}{\hbar}\omega_c(n+\frac{1}{2})$ labelled with the quantum number n. Therefore, a level consists of those states which were located between the circumference of the level taken into consideration, and the subsequent one (right image in figure 5.1).

So the degeneracy of a level can be calculated by dividing the area of an annulus by the area that each state occupied

$$g = \frac{\pi \frac{2m}{\hbar^2}\left(\hbar\omega_c(n+3/2) - \hbar\omega_c(n+1/2)\right)}{\left(\frac{2\pi}{L}\right)^2} = \frac{eHL^2}{2\pi\hbar c} \tag{5.5}$$

Fixing the energy ϵ, and adding the possibility for k_z to assume all the values $k_z = \frac{2\pi n_z}{L}$ compatible with this energy, we obtained the *Landau tubes* represented in figure 5.2.

Chapter 6

Landau's approach

6.1 Landau's derivation of diamagnetism

Now, we will follow Landau's original way of deriving the diamagnetism of a free electron gas. We consider our system in the limit of weak field H.

First we calculate the spin-field coupling contribution to the magnetic susceptibility. The grand canonical potential of a free electron gas is, thanks to the relation (2.11)

$$\Omega_0 = -\frac{2}{\beta}\sum_{n_x\in\mathbb{Z}}\sum_{n_y\in\mathbb{Z}}\sum_{n_z\in\mathbb{Z}}\ln\left(1+e^{-\beta(\frac{\hbar^2k^2}{2m^*}-\mu)}\right)$$

where the factor 2 is due to the spin degeneracy of each state. Multiplying and dividing by $\Delta k_i = \frac{2\pi}{L}$, for $i = x, y, z$ we can approximate the last sum with an integral thanks to the fact that the box considered has $L \gg 1$. In fact it becomes

$$\Omega_0 = -\frac{2}{\beta}\left(\frac{L}{2\pi}\right)^3\int_{-\infty}^{+\infty}dk_x\int_{-\infty}^{+\infty}dk_y\int_{-\infty}^{+\infty}dk_z\ln\left(1+e^{-\beta(\frac{\hbar^2k^2}{2m^*}-\mu)}\right)$$

and changing to spherical coordinates in k space we obtain

$$\Omega_0(\mu) = -\frac{V}{\beta\pi}\int_0^{\infty}dk\ln\left(1+e^{-\beta(\frac{\hbar^2k^2}{2m^*}-\mu)}\right)$$

Including in the Hamiltonian the spin-field coupling contribution cancels the 2 factor of the spin degeneracy and makes a translation of the chemical potential, that is

$$\Omega_{par} = \frac{1}{2}\left(\Omega_0(\mu-\mu_B H)+\Omega_0(\mu+\mu_B H)\right)$$

This leads to a second order H correction

$$\Omega_{par} = \Omega_0 + \frac{\mu_B^2H^2}{2}\frac{\partial^2\Omega_0}{\partial\mu^2} + o(H^2)$$

and a contribution to the magnetic susceptibility

$$\chi_{par} = -\frac{\mu_B^2}{V}\frac{\partial^2\Omega_0}{\partial\mu^2} = \frac{\mu_B^2}{V}\rho(\epsilon_F) \tag{6.1}$$

where in we have substituted the relation (B.4) of appendix B.2 and we have identified $\epsilon_F = \mu$ in the limit of $T = 0$.

On the other hand, including in the Hamiltonian the Landau levels contribution maintains the spin degeneracy factor and the grand canonical potential, thanks to the relation (2.11), becomes

$$\Omega_{dia} = -\frac{2}{\beta}\sum_{n=0}^{+\infty}\sum_{n_z\in\mathbb{Z}}\frac{eHL^2}{2\pi\hbar c}\ln\left(1+e^{-\beta(\epsilon_{nn_z}-\mu)}\right)$$

Taking the limit to continuum we can write

$$\Omega_{dia} = -\frac{eHV}{\beta 2\pi^2\hbar c}\sum_{n=0}^{\infty}\int_{-\infty}^{+\infty}dk_z\ln\left(1+e^{-\beta\left(\frac{\hbar^2k_z^2}{2m^*}+\hbar\omega_c\left(n+\frac{1}{2}\right)-\mu\right)}\right)$$

To make this calculation, Landau used the Euler-Maclaurin summation formula

$$\sum_{n=0}^{+\infty}F(n+\frac{1}{2}) \approx \int_0^{+\infty}F(x)dx + \frac{1}{24}F'(0) \tag{6.2}$$

which is a reasonable approximation in the limit in which F makes a small variation when evaluated in two consecutive Landau levels. This is equivalent to the condition $\beta\hbar\omega_c \ll 1$, which will also be assumed in Peierls' derivation (7.1).

Proceeding we obtain

$$\Omega_{dia} = -\frac{eHV}{\beta 2\pi^2\hbar c}\int_0^{+\infty}dx\int_{-\infty}^{+\infty}dk_z\ln\left(1+e^{-\beta\left(\frac{\hbar^2k_z^2}{2m^*}+\hbar\omega_c x-\mu\right)}\right)+$$

$$-\frac{1}{24}\frac{eHV}{\beta 2\pi^2\hbar c}\int_{-\infty}^{+\infty}dk_z\frac{-\beta\hbar\omega_c}{1+e^{\beta\left(\frac{\hbar^2k_z^2}{2m^*}-\mu\right)}}$$

Changing tha variable $\mu' \to \mu - \hbar\omega_c x$ in the first integral makes the first addend independent from H, so it can be identified with Ω_0. The second addend can be recognised as a factor times the second derivative of the first addend with respect to μ.

In particular, using the relations $\omega_c = \frac{eH}{m^*c}$ and $\mu_B = \frac{e\hbar}{2mc}$ we can write

$$\Omega_{dia} = \Omega_0 - \frac{\hbar^2\omega_c^2}{24}\frac{\partial^2\Omega_0}{\partial\mu^2} = \Omega_0 - \frac{\mu_B^2H^2}{6}\left(\frac{m}{m^*}\right)^2\frac{\partial^2\Omega_0}{\partial\mu^2}$$

and in the end we obtain

$$\chi_{dia} = -\frac{\mu_B^2}{3V}\left(\frac{m}{m^*}\right)^2\frac{\partial^2\Omega_0}{\partial\mu^2} = -\frac{1}{3}\left(\frac{m}{m^*}\right)^2\chi_{par} \tag{6.3}$$

where we have recognised equation (6.1). χ_{par} can be derived analytically with standard techniques.

6.2 Simplified model of de Haas-van Alphen oscillations

To understand the underlying principle of this phenomenon, we take a 2D free electron gas, composed of N electrons at zero temperature in a very strong magnetic field. The zero temperature limit implies that the occupation of the levels, as a function of the energy, is a Heaviside Θ as it will be discussed in the Peierls' method chapter.

Trying to make a more rigorous sense to the expression "very strong", we call H_0 a field such that all electrons lie in the ground state (first Landau level). Recalling equation (5.5), the degeneracy of each Landau level is $g = \frac{AeH}{\pi\hbar c}$ (there is an extra factor 2 due to spin degeneracy), hence $H_0 = \frac{N\pi\hbar c}{Ae}$.

Since $T = 0$, for $H > H_0$ every electron lies in the ground state and the total energy of the gas is simply N times the energy of the ground state, that is $E_0 = N\epsilon_0 = N\frac{\hbar\omega_c}{2}$.

Instead, if $H < H_0$, there exists a number $\overline{n}$ such that the $\overline{n}$-th Landau level is completely full and the $\overline{n}+1$-th Landau level can be from empty to almost full. This is represented by the condition $(\overline{n}+1)g < N < (\overline{n}+2)g$, and substituting the expression for g it becomes $\frac{1}{\overline{n}+1} < \frac{H}{H_0} < \frac{1}{\overline{n}+2}$. The total energy of such a system can be calculated by summing the energy of every electron. $(\overline{n}+1)g$ of them lie in Landau levels with energy $\epsilon_n = \hbar\omega_c(n+\frac{1}{2})$ for $n = 0, 1, ..., \overline{n}$ and the remaining $N - (\overline{n}+1)g$ electrons have energy $\epsilon_{\overline{n}+1} = \hbar\omega_c(\overline{n}+\frac{3}{2})$. Therefore we obtained the total energy

$$E = g\sum_{n=0}^{\overline{n}} \hbar\omega_c(n+\frac{1}{2}) + (N-(\overline{n}+1)g)\hbar\omega_c(\overline{n}+\frac{3}{2})$$

which can be elaborated in the form

$$E = \frac{Ne\hbar}{mc}\left[\frac{H}{H_0}\left(\overline{n}+\frac{3}{2}\right) - \frac{(\overline{n}+1)(\overline{n}+2)}{2}\frac{H^2}{H_0^2}\right]$$

The magnetization and the magnetic susceptibility can be derived from the already mentioned formulas $M = -\frac{1}{V}\frac{\partial E}{\partial H}$ and $\chi = \frac{\partial M}{\partial H}$. Substituting the constant $\mu_B = \frac{e\hbar}{2mc}$, we find the following functions (represented in figure 6.1)

$$M = \begin{cases} -\mu_B\frac{N}{V} & H > H_0 \\ \mu_B\frac{N}{V}\left[2(\overline{n}+1)(\overline{n}+2)\frac{H}{H_0} - (2\overline{n}+3)\right] & \frac{1}{\overline{n}+2} < \frac{H}{H_0} < \frac{1}{\overline{n}+1} \end{cases} \tag{6.4}$$

$$\chi = \begin{cases} 0 & H > H_0 \\ \mu_B\frac{N}{V}\left[2(\overline{n}+1)(\overline{n}+2)\frac{H}{H_0} - (2\overline{n}+3)\right] & \frac{1}{\overline{n}+2} < \frac{H}{H_0} < \frac{1}{\overline{n}+1} \end{cases} \tag{6.5}$$

It is then evident the oscillatory behaviour in the magnetization and its interpretation.

In fact, starting from a H_0 field, all electrons lie in the ground state. The moment the condition $H < H_0$ is fulfilled, electrons are excited to the $n = 1$ state, beacuse there is no more space for them in the ground state.

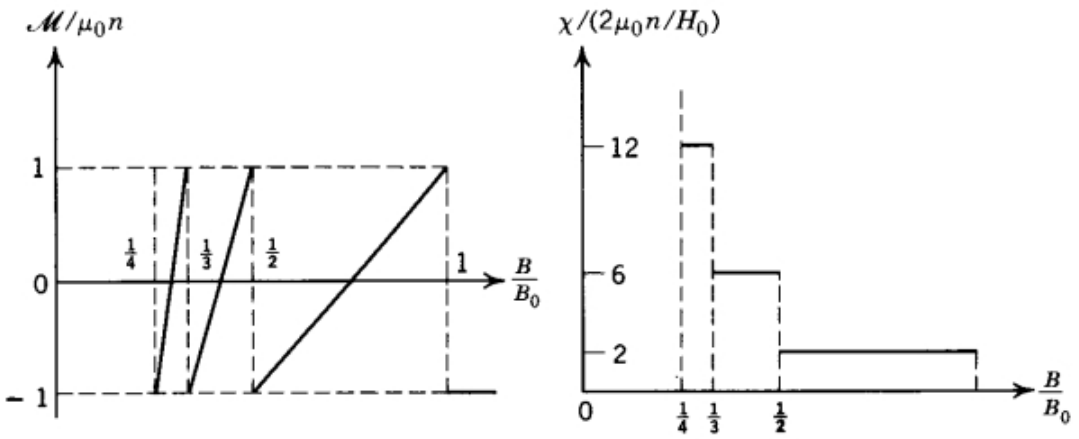

Figure 6.1: Magnetization and magnetic susceptibility in an electron gas at $T = 0$, as functions of the magnetic field strength B. *Meccanica Statistica*, K. Huang, 1997.

So the variation of energy due to the decreasing in the field is composed of 2 factor: the energy of each state decreases with the field, but some electrons increase their energy moving to the above level. Of these 2 contributions, at the beginning the excitations of the electrons has a bigger effect and it raises the total energy (negative value of the magnetization), but then the lowering of the energy states takes over (the magnetization value increases till it becomes positive) and when also the second level is filled, the energy is back to the value we started with.

Lowering further the field makes what said above to start over, and it makes the magnetization to quickly change (at $T = 0$ instantly) from a positive to a negative value. M can be viewed as an oscillating function in $\frac{1}{H}$ with period $\frac{1}{H_0}$.

Chapter 7

Peierls' method

The following derivations are aimed to describe the motion of the electrons inside a metal immersed in a uniform magnetic field in order to identify some characteristics when the system is under certain conditions. The effects analysed are Pauli paramagnetism, Landau diamagnetism and de Haas-van Alphen oscillations of the magnetization.

The value range for the magnetic field is

$$\epsilon_F \gg \hbar\omega_c \gg k_B T \tag{7.1}$$

The physical meaning of this assumption is that there is an almost continuous structure of Landau levels that electrons can occupy up to the Fermi energy and that very few electrons occupy energy levels over the Fermi energy, so the statistic of the electrons is almost the one of a Fermi gas ($T = 0$).

7.1 Mathematics behind the method

To avoid the difficulty of deriving directly from the definition the grand canonical potential, Peierls' method exploits the relation of this quantity with Boltzmann partition function, which can be obtained exactly by an analitical calculation.

In particular, considering equation (2.11)

$$\Omega = -\frac{1}{\beta}\sum_a g_a \ln\left(1 + e^{-\beta(\epsilon_a - \mu)}\right)$$

it is useful to call

$$F(\epsilon) := -\frac{1}{\beta}\ln\left(1 + e^{-\beta(\epsilon-\mu)}\right)$$

so that $\Omega = \sum_a g_a F(\epsilon_a)$ and we can recognise that $F(\epsilon)$ is indeed the primitive of the Fermi-Dirac distribution of the density of states $f(\epsilon) = \frac{1}{1+e^{\beta(\epsilon-\mu)}}$ represented in figure 7.1.

We denote the Laplace transform of $F(\epsilon)$ by

$$\tilde{F}(s) = \mathscr{L}[F](s) = \int_0^{+\infty} e^{-s\epsilon} F(\epsilon)\, d\epsilon$$

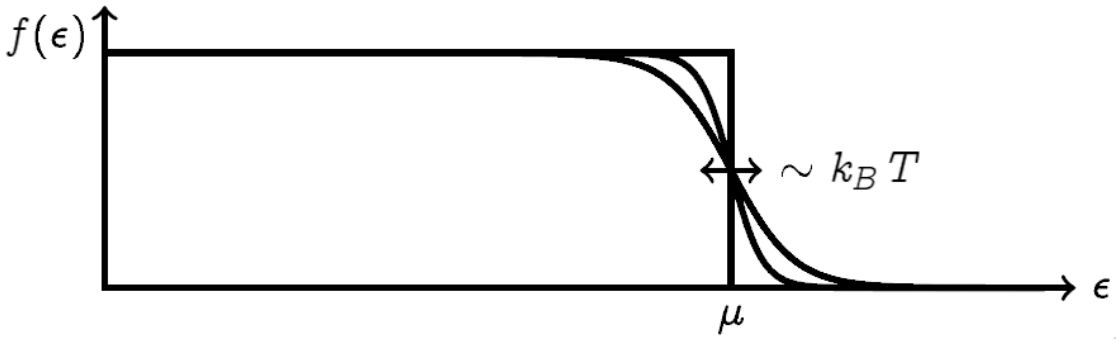

Figure 7.1: Fermi-Dirac distribution of the density of states $f(\epsilon) = \frac{1}{1+e^{\beta(\epsilon-\mu)}}$

and the Laplace antitransform (Laplace inversione theorem)

$$\mathscr{L}^{-1}[\tilde{F}](\epsilon) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{s\epsilon} \tilde{F}(s) = \begin{cases} F(\epsilon) & \epsilon > 0 \\ 0 & \epsilon < 0 \end{cases}$$

with $c \in \mathbb{R}$ and such that it is greater than the real part of every pole of $\tilde{F}$. So we write

$$\Omega = \sum_a g_a \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{s\epsilon_a} \tilde{F}(s)$$

and here we substitute the single particle Boltzmann partition function (2.7), where we allow the β coefficient to assume complex values $Z(s) = \sum_a g_a e^{-s\epsilon_a}$, obtaining

$$\Omega = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \tilde{F}(s) s^2 \frac{Z(-s)}{s^2} =$$

Now we define $\tilde{A}(s) := \tilde{F}(s)s^2$ and $\tilde{B}(s) := \frac{Z(s)}{s^2}$ and using the formula for the resultant (proof in appendix A.1)

$$= \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \tilde{A}(s)\tilde{B}(-s) = \int_0^{+\infty} A(\epsilon)B(\epsilon)\, d\epsilon$$

the problem reduces to the calculation of

$$A(\epsilon) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{s\epsilon} \tilde{F}(s) s^2 = \frac{d^2F(\epsilon)}{dE^2} = \frac{df(\epsilon)}{d\epsilon}$$

$$B(\epsilon) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{s\epsilon} \frac{Z(s)}{s^2}$$

7.2 2D derivation

7.2.1 Boltzmann partition function

The first task is now to obtain explicitly the single particle Boltzmann partition function. Recalling the relation (2.7)

$$Z = \sum_a g_a e^{-\beta\epsilon_a} = \sum_{m_s n} g e^{-\beta\epsilon_{m_s n}}$$

and the degeneracy of each Landau level (5.5) $g = \frac{AeH}{2\pi\hbar c}$, the eigenvalues of the single particle Hamiltonian are

$$\epsilon = \hbar\omega_c(n + \frac{1}{2}) + m_s\mu_B H \tag{7.2}$$

Calculating the sum over the quantum numbers

$$Z = \frac{AeH}{2\pi\hbar c} \sum_{m_s=-1}^{1} e^{-\beta m_s \mu_B H} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega_c(n+1/2)}$$

leads to

$$Z(\beta) = \frac{AeH}{2\pi\hbar c} \frac{\cosh(\beta\mu_B H)}{\sinh\left(\frac{\beta\hbar\omega_c}{2}\right)} \tag{7.3}$$

Now we substitute $Z(s)$ in the formula for $B(E)$ obtaining

$$B(\epsilon) = \frac{AeH}{2\pi\hbar c} \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \frac{e^{s\epsilon}}{s^2} \frac{\cosh(s\mu_B H)}{\sinh\left(\frac{s\hbar\omega_c}{2}\right)}$$

We change variables into the simpler units $z := \frac{s\hbar\omega_c}{2}$ and $x := \frac{2\epsilon}{\hbar\omega_c}$, for which $z \gg 1$ and $x \gg 1$ hold because of approximation (7.1), so that it becomes

$$B = \left(\frac{AeH}{2\pi\hbar c}\right)\left(\frac{\hbar\omega_c}{2}\right) I(x) \tag{7.4}$$

where

$$I(x) = \int_{c-i\infty}^{c+i\infty} \frac{dz}{2\pi i} \frac{e^{zx}}{z^2} \frac{\cosh\left(z\frac{m^*}{m}\right)}{\sinh z} \tag{7.5}$$

7.2.2 The integral in 2D

The integral $I(x)$ is along the vertical line of real part c in the complex plane. This line can be viewed as the limit for $M \to \infty$ of the segment with endpoints $(c, -iM)$ and $(c, +iM)$. Therefore, taking into consideration the presence of poles on the imaginary axe, we connect the segment endpoints to get the path in figure 7.2.

We can now apply the residue theorem and obtain $I(x) + I_{SC} = \sum \text{Res}$, where I_{SC} is the integral along the semicircumference followed counter clockwise, and $\sum Res$ is the sum over the poles of the residues of the integrand.

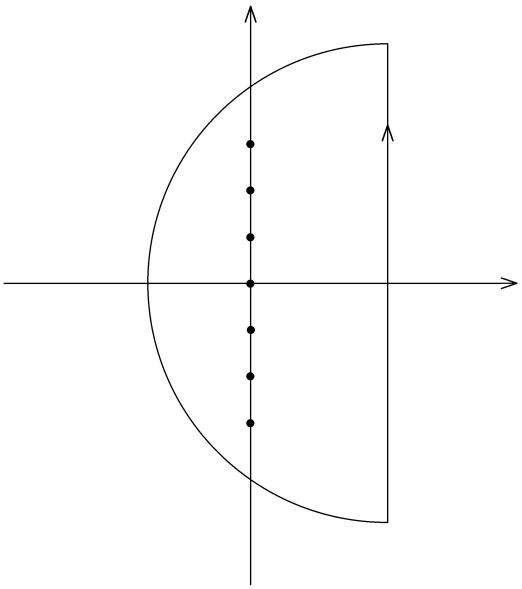

Figure 7.2: It is represented the path which is followed during the integration.

Beacuse of $\sinh z$ term in the denominator, there are infinite simple poles of the form $n\pi i$ for $n \in \mathbb{Z}$ and because of z^2 term, the pole in $z = 0$ becomes of third order. I_{sc} vanishes in the limit of $M \to \infty$, so to evaluate the integral we need to calculate the sum of the residues. The pole in the origin contribution can be identified with Pauli paramagnetism and Landau diamagnetism, and the other poles contribution with the de Haas-van Alphen effect.

7.2.3 Pauli paramagnetism and Landau diamagnetism

We proceed with the evaluation of

$$\mathrm{Res}\left(\frac{e^{zx}}{z^2}\frac{\cosh\left(z\frac{m^*}{m}\right)}{\sinh z}, z=0\right)$$

Laurent expanding the function in $z = 0$ and obtaining the residue as the coefficient of the $\frac{1}{z}$ term of the serie.

In particular we write

$$\frac{1}{z^2}\left(\frac{1}{z+\frac{z^3}{6}+O(z^4)}\right)\left(1+xz+\frac{x^2z^2}{2}+O(z^3)\right)\left(1+\frac{(m^*)^2z^2}{2m^2}+O(z^3)\right)=$$

$$=\frac{1}{z^3}+\frac{x}{z^2}+\frac{1}{2z}\left(x^2+\left(\frac{m^*}{m}\right)^2-\frac{1}{3}\right)+O(1)$$

which leads to $\mathrm{Res}_{z=0} = \frac{1}{2}\left(x^2+\left(\frac{m^*}{m}\right)^2-\frac{1}{3}\right)$.

$A(\epsilon)$ is the derivative of the Fermi-Dirac distribution and in the limit of low temperature $f(\epsilon) \to \Theta(\mu - \epsilon)$, so $A(\epsilon) \to -\delta(\epsilon - \mu)$, while $B(\epsilon)$ is slowly varying with the energy, therefore we calculate

$$\Omega = -B(\mu) = \Omega_0 - \frac{Am^*}{2\pi\hbar^2}\mu_B^2 H^2 \left(1 - \frac{1}{3}\left(\frac{m}{m^*}\right)^2\right) \tag{7.6}$$

where

$$\Omega_0 = -\frac{Am^*\mu^2}{2\pi\hbar^2}$$

is the grand canonical potential of a 2D free electron gas (obtained in appendix B.1) and it is H independent.

There is no difference between the chemical potential μ and the Fermi energy ϵ_F of a 2D free electron gas (obtained in appendix B.1). In fact, since the magnetic correction to the grand canonical potential is independent from μ, imposing the average value of the number of electrons N for the free electron gas and for our system thanks to the relation $N = -\frac{\partial\Omega}{\partial\mu}$, implies that $\mu = \epsilon_F$. Therefore the magnetization and the magnetic scusceptibility are

$$M = \mu_B^2 H \rho(\epsilon_F)\left[1 - \frac{1}{3}\left(\frac{m}{m^*}\right)^2\right] \tag{7.7}$$

$$\chi = \mu_B^2 \rho(\epsilon_F)\left[1 - \frac{1}{3}\left(\frac{m}{m^*}\right)^2\right] \tag{7.8}$$

where $\rho(\epsilon_F)$ is the density of states at the Fermi energy for the free electron gas (obtained in appendix B.1).

7.2.4 The de Haas-van Alphen effect

Here we derive the contribution of the poles to grand canonical potential

$$\sum \mathrm{Res} = \sum_{\substack{n\in\mathbb{Z}\\ n\neq 0}} \lim_{z\to n\pi i}(z - n\pi i)\frac{e^{zx}\cosh\left(z\frac{m^*}{m}\right)}{z^2\sinh z} =$$

$$= -\sum_{\substack{n\in\mathbb{Z}\\ n\neq 0}} \lim_{t\to n\pi} \frac{(t - n\pi)e^{in\pi x}\cos(n\pi\frac{m^*}{m})}{(n\pi)^2\sin(t)} =$$

calculating the limit we obtain

$$= -\sum_{\substack{n\in\mathbb{Z}\\ n\neq 0}} \frac{(-)^n}{(n\pi)^2} e^{in\pi x}\cos\left(n\pi\frac{m^*}{m}\right) =$$

In the sum only even function contribute, hence

$$= -2\sum_{n=1}^{+\infty}(-)^n\frac{\cos(xn\pi)}{(n\pi)^2}\cos\left(\frac{m^*}{m}n\pi\right)$$

In this case, we can not approximate $A(\epsilon)$ with the Dirac delta function since $B(\epsilon)$ is a quickly varying function with respect to the energy, so we have to calculate the integral before taking the low temperature limit. In particular

$$\Omega = \left(\frac{\beta AeH}{4\pi\hbar c}\right)\left(\frac{\hbar\omega_c}{2}\right)\sum_{n=1}^{+\infty}(-)^n\frac{\cos(\frac{m^*}{m}n\pi)}{(n\pi)^2}\int_0^{+\infty}d\epsilon\frac{\cos\left(\frac{n\pi 2\epsilon}{\hbar\omega_c}\right)}{\cosh^2\left(\beta\frac{\epsilon-\mu}{2}\right)}$$

Making the substitution $t := \beta\frac{\epsilon-\mu}{2}$ allow us to recognise a known integral and to clarify what is involved in the limit $T \to 0$. So we obtain

$$\Omega = \left(\frac{AeH}{2\pi\hbar c}\right)\left(\frac{\hbar\omega_c}{2}\right)\sum_{n=1}^{+\infty}(-)^n\frac{\cos(\frac{m^*}{m}n\pi)}{(n\pi)^2}\cos\left(\frac{2n\pi\mu}{\hbar\omega_c}\right)J$$

where J is the following integral (calculated in appendix A.3)

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

where, since $\mu \gg k_B T$ thanks to the approximation (7.1), we have extended the integral till $-\infty$. In the end we elaborate the grand canonical potential in the form

$$\Omega = \frac{AeH}{\pi\hbar c\beta}\sum_{n=1}^{+\infty}\frac{(-)^n}{n}\cos\left(n\pi\frac{m^*}{m}\right)\frac{\cos\left(\frac{2n\pi\mu}{\hbar\omega_c}\right)}{\sinh\left(\frac{2n\pi^2}{\beta\hbar\omega_c}\right)} \tag{7.9}$$

It appears evident that the magnetization can be viewed as an oscillating function of the variable $\frac{1}{H}$ with fundamental (shortest) period $\Delta\left(\frac{1}{H}\right) = \frac{e\hbar}{\epsilon_F m^* c}$. This result is coherent with the simplified ($T = 0$) derivation already done, where we found $\Delta\left(\frac{1}{H}\right) = \frac{1}{H_0} = \frac{Ae}{N\pi\hbar c}$. These 2 expression coincide if we substitute $N = \frac{m^*\epsilon_F A}{\pi\hbar^2}$ the number of electrons for a $T = 0$ electron gas.

7.3 3D derivation

7.3.1 Boltzmann partition function

The first task is again to obtain explicitly the single particle Boltzmann partition function. Recalling the relation (2.7)

$$Z = \sum_a g_a e^{-\beta\epsilon_a} = \sum_{m_s n k_z} g e^{-\beta\epsilon_{m_s n k_z}}$$

and introducing the degeneracy of each Landau level $g = \frac{AeH}{2\pi\hbar c}$, the eigenvalues of the single particle Hamiltonian are

$$\epsilon = \frac{\hbar^2 k_z^2}{2m^*} + \hbar\omega_c(n + \frac{1}{2}) + m_s\mu_B H \tag{7.10}$$

Taking the limit to continuum as done above we write

$$Z = \frac{VeH}{4\pi^2\hbar c} \sum_{m_s=-1}^{1} e^{-\beta m_s \mu_B H} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega_c(n+1/2)} \int_{-\infty}^{+\infty} dk_z e^{-\beta\frac{\hbar^2 k_z^2}{2m^*}}$$

which leads to

$$Z(\beta) = \frac{VeH}{2\pi\hbar c}\left(\frac{m^*}{2\pi\hbar^2\beta}\right)^{\frac{1}{2}} \frac{\cosh(\beta\mu_B H)}{\sinh\left(\frac{\beta\hbar\omega_c}{2}\right)} \tag{7.11}$$

Now we substitute $Z(s)$ in the formula for $B(\epsilon)$ obtaining

$$B(\epsilon) = \frac{VeH}{2\pi\hbar c}\left(\frac{m^*}{2\pi\hbar^2}\right)^{\frac{1}{2}} \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \frac{e^{s\epsilon}}{s^{3/2}} \frac{\cosh(s\mu_B H)}{\sinh\left(\frac{s\hbar\omega_c}{2}\right)}$$

We change variables into the simpler units $z := \frac{s\hbar\omega_c}{2}$ and $x := \frac{2\epsilon}{\hbar\omega_c}$, for which $z \gg 1$ and $x \gg 1$ hold thanks to approximation (7.1), so that it becomes

$$B(x) = 2V\left(\frac{m^*}{2\pi\hbar^2}\right)^{\frac{3}{2}}\left(\frac{\hbar\omega_c}{2}\right)^{\frac{5}{2}} I(x) \tag{7.12}$$

where

$$I(x) = \int_{c-i\infty}^{c+i\infty} \frac{dz}{2\pi i} e^{zx} \frac{\cosh\left(z\frac{m^*}{m}\right)}{z^{5/2}\sinh z} \tag{7.13}$$

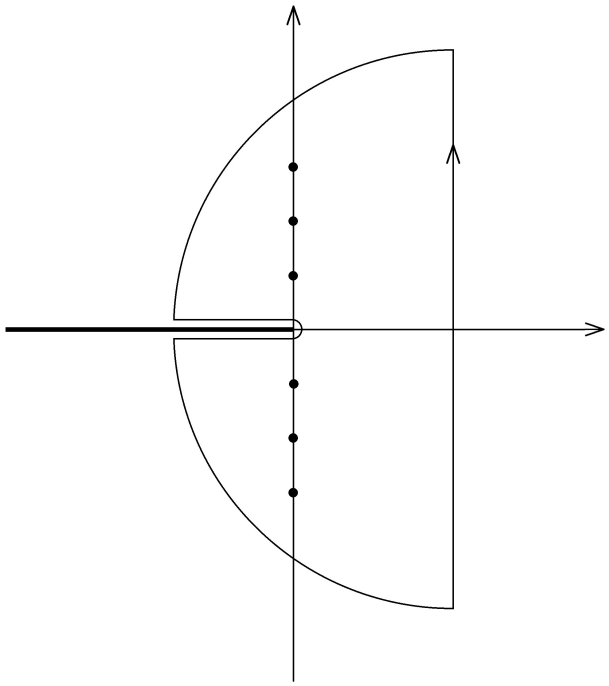

Figure 7.3: It is represented the path which is followed during the integration. We refer to σ as the key hole path followed in the opposite direction compared to this figure

7.3.2 The integral in 3D

The integral $I(x)$ is along the vertical line of real part c in the complex plane. This line can be viewed as the limit for $M \to \infty$ of the segment with endpoints $(c, -iM)$ and $(c, +iM)$. Therefore, taking into consideration the presence of the branch in the negative real axe, we connect the segment endpoints to get the path in figure 7.3.

We can now apply the residue theorem and obtain $I(x)+I_{SC}+I_{sc} = I_\sigma+\sum \text{Res}$, where I_σ is the path along the key-hole followed clockwise, I_{SC} is the integral along the outer semicircumference followed counter clockwise, I_{sc} is the integral along the inner semicircumference fllowed clockwisen and $\sum \text{Res}$ is the sum over the poles of the residues of the integrand.

In the case of sinh, these are $n\pi i$ for $n \in \mathbb{Z}$ but $n \neq 0$ since it is outside the path. I_{sc} vanishes in the limit of $M \to \infty$, so the only 2 addens left are I_σ, which can be identified with Pauli paramagnetism and Landau diamagnetism contribution, and $\sum \text{Res}$, which is the contribution of the de Haas-van Alphen effect.

7.3.3 Pauli paramagnetism and Landau diamagnetism

We proceed with the evaluation of

$$I_\sigma = \int_\sigma \frac{dz}{2\pi i} \frac{e^{zx}}{z^{5/2}} \frac{\cosh\left(z\frac{m^*}{m}\right)}{\sinh z} = \frac{1}{2}\int_\sigma \frac{dz}{2\pi i} \frac{e^{z\left(x+\frac{m^*}{m}\right)} + e^{z\left(x-\frac{m^*}{m}\right)}}{z^{5/2}\sinh z}$$

expanding the denominator in $z = 0$ (as it will be explained, only the first 2 orders give rise to non neglectable terms) we can write

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

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

$$\int_\sigma \frac{dz}{2\pi i} e^{zx}\cosh\left(z\frac{m^*}{m}\right) O(\sqrt{z})$$

We can recognise Hankel representation of Euler Γ function (proof in appendix A.2)

$$\frac{1}{\Gamma(\alpha)} = \int_\sigma \frac{dz}{2\pi i} e^z z^{-\alpha} \tag{7.14}$$

and the last addend is $O(x^{-3/2})$, therefore, since $x \gg 1.$, taking into consideration higher order terms in sinh expansion will generate neglectable addends. Substituting $\Gamma(\frac{7}{2}) = \frac{15\sqrt{\pi}}{8}$ and $\Gamma(\frac{5}{2}) = \frac{\sqrt{\pi}}{2}$ and developing the expansion, we obtain

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

$A(\epsilon)$ is the derivative of the Fermi-Dirac distribution and in the limit of low temperature $f(\epsilon) \to \Theta(\mu - \epsilon)$, so $A(\epsilon) \to -\delta(\epsilon - \mu)$ while $B(\epsilon)$ is slowly varying with the energy, so in the end we calculate

$$\Omega = -B(\mu) = \Omega_0 - \frac{2V}{\sqrt{\pi}}\left(\frac{m^*}{2\pi\hbar^2}\right)^{3/2}\mu_B^2 H^2\sqrt{\mu}\left(1 - \frac{1}{3}\left(\frac{m}{m^*}\right)^2\right) \tag{7.15}$$

where

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

is the grand canonical potential of a 3D free electron gas (obtained in appendix B.2) and it is H independent.

The difference between the chemical potential μ and the Fermi energy E_F of a free electron gas (obtained in appendix B.2) can be neglected. In fact, imposing the average value of the number of electrons N for the free electron gas and for our system, and thanks to the relation $N = -\frac{\partial\Omega}{\partial\mu}$, we derive the equation

$$\frac{\mu}{\epsilon_F} = 1 - \frac{\mu_B^2 H^2}{4\sqrt{\mu}\epsilon_F^{3/2}}\left(1 - \frac{1}{3}\left(\frac{m}{m^*}\right)^2\right)$$

where we can see that the correction is approximately of second order in $\frac{\hbar\omega_c}{\epsilon_F}$.

Therefore the magnetization and the magnetic scusceptibility are

$$M = \mu_B^2 H \rho(\epsilon_F) \left[1 - \frac{1}{3}\left(\frac{m}{m^*}\right)^2\right] \tag{7.16}$$

$$\chi = \mu_B^2 \rho(\epsilon_F) \left[1 - \frac{1}{3}\left(\frac{m}{m^*}\right)^2\right] \tag{7.17}$$

where $\rho(\epsilon_F)$ is the density of states at the Fermi energy for the free electron gas (obtained in appendix B.2). This is the same result obtained by Landau in his treatment.

7.3.4 The de Haas-van Alphen effect

Here we derive the contribution of the poles to the grand canonical potential

$$\sum \mathrm{Res} = \sum_{\substack{n\in\mathbb{Z}\\ n\neq 0}} \lim_{z\to n\pi i} (z - n\pi i) \frac{e^{zx}\cosh\left(z\frac{m^*}{m}\right)}{z^{5/2}\sinh(z)} =$$

$$= \sum_{\substack{n\in\mathbb{Z}\\ n\neq 0}} \lim_{t\to n\pi} \frac{(t - n\pi) e^{in\pi x}\cos(n\pi\frac{m^*}{m})}{e^{\frac{5}{2}(\ln(n\pi)+i\pi/2)}\sin(t)} =$$

Calculating the limit we obtain

$$= -\sum_{\substack{n\in\mathbb{Z}\\ n\neq 0}} \frac{(-)^n}{(n\pi)^{5/2}} e^{i(n\pi x - \pi/4)} \cos\left(n\pi\frac{m^*}{m}\right) =$$

In the sum only even function contribute, hence

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

In this case, we can not approximate $A(\epsilon)$ with the Dirac delta function since $B(\epsilon)$ is a quickly varying function with respect to the energy, so we have to calculate the integral before taking the low temperature limit. In particular

$$\Omega = \beta V \left(\frac{m^*}{2\pi\hbar^2}\right)^{3/2} \left(\frac{\hbar\omega_c}{2}\right)^{5/2} \sum_{n=1}^{+\infty} (-)^n \frac{\cos(\frac{m^*}{m} n\pi)}{(n\pi)^{5/2}} \int_0^{+\infty} d\epsilon \frac{\cos\left(\frac{2n\pi\epsilon}{\hbar\omega_c} - \frac{\pi}{4}\right)}{\cosh^2\left(\beta\frac{\epsilon-\mu}{2}\right)}$$

Making the substitution $t := \beta\frac{\epsilon-\mu}{2}$ allow us to recognise a known integral and to clarify what is involved in the limit $T \to 0$.

So we obtain

$$\Omega = 2V \left(\frac{m^*}{2\pi\hbar^2}\right)^{3/2} \left(\frac{\hbar\omega_c}{2}\right)^{5/2} \sum_{n=1}^{+\infty} (-)^n \frac{\cos(\frac{m^*}{m} n\pi)}{(n\pi)^{5/2}} \cos\left(\frac{2n\pi\mu}{\hbar\omega_c} - \frac{\pi}{4}\right) J$$

where J is the following integral (calculated in appendix A.3)

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

where, since $\mu \gg k_B T$, we have extended the integral till $-\infty$. In the end we elaborate the grand canonical potential in the form

$$\Omega = \frac{V}{2\pi^2\beta}\left(\frac{eH}{\hbar c}\right)^{3/2} \sum_{n=1}^{+\infty} \frac{(-)^n}{n^{3/2}} \cos\left(n\pi\frac{m^*}{m}\right) \frac{\cos\left(\frac{2n\pi\mu}{\hbar\omega_c} - \frac{\pi}{4}\right)}{\sinh\left(\frac{2\pi^2 n}{\beta\hbar\omega_c}\right)} \tag{7.18}$$

7.4 Comparing semiclassical and quantum results

In the limit (7.1), we can identify μ with the ϵ_F of a free electron gas and it appears evident that the magnetization, both in 2D e 3D, oscillates as a function of $\frac{1}{H}$ with fundamental period $\Delta\left(\frac{1}{H}\right) = \frac{e\hbar}{m^* c\epsilon_F}$. This result is coherent with the semiclassical one (4.13) $\Delta\left(\frac{1}{H}\right) = \frac{2\pi e}{\hbar c S_{ex}(\epsilon_F)}$.

Thanks to Onsager relation (4.11) $S_n(\epsilon, k_z) = \Delta S(\epsilon, k_z)\left(n + \frac{1}{2}\right)$, there exist an $\bar{n}$ such that $S_{ex}(\epsilon_F) = \Delta S_{ex}(\epsilon_F)\left(\bar{n} + \frac{1}{2}\right)$. We can now approximate $\Delta S_{ex}(\epsilon_F) \cong \left.\frac{\partial S_{ex}(\epsilon)}{\partial\epsilon}\right|_{\epsilon=\epsilon_F} \Delta\epsilon$ where, since our Fermi surface is assumed to be almost spherical we obtain $k_{zex} = 0$, hence $\Delta\epsilon = \hbar\omega_c$ and $\epsilon_F = \left(\bar{n} + \frac{1}{2}\right)\Delta\epsilon$.

Therefore, the relation we obtain is $S_{ex}(\epsilon_F) = \left.\frac{\partial S_{ex}(\epsilon)}{\partial\epsilon}\right|_{\epsilon=\epsilon_F} \epsilon_F$ where, in the partial derivative, we can recognise the definition of the effective mass $m^*(\epsilon_F, k_{zex}) = \frac{\hbar^2}{2\pi}\left.\frac{\partial S_{ex}(\epsilon)}{\partial\epsilon}\right|_{\epsilon=\epsilon_F}$, evaluated at ϵ_F and k_{zex}.

Making this substitution, the 2 periods coincide. The semiclassical period is more general than the one found by Peierls' method for an almost free electron gas, since it can take into account not only ellipsoid Fermi surfaces, but very different shapes.

Appendix A

A.1 Proof of the resultant formula

Here we provide a proof to the resultant formula, which is

$$\int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \tilde{A}(s)\tilde{B}(-s)e^{sx} = \int_{\max(0,x)}^{+\infty} d\epsilon\, A(\epsilon)B(\epsilon - x) \tag{A.1}$$

where $\tilde{A}(s) = \mathscr{L}[A](s)$ and $\tilde{B}(s) = \mathscr{L}[B](s)$.

Replacing $\tilde{B}(s)$ with the definition of the Laplace transform we obtain for the first term

$$\int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \tilde{A}(s)e^{sx} \int_0^{+\infty} dy\, B(y)e^{sy} = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \int_0^{+\infty} dy B(y)\tilde{A}(s)e^{s(x+y)}$$

We can now interchange the integrals and recognise the Laplace antitrasform of $\tilde{A}(s)$ and substitute it

$$\int_0^{+\infty} dy\, B(y) \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \tilde{A}(s)e^{s(y+x)} = \int_0^{+\infty} dy\, B(y)A(y+x)\Theta(y+x)$$

which gives the expressione above after the variable change $E := x + y$.

A.2 Hankel representation of Euler Γ function

Here we provide a proof to the formula known as Hankel representation of Euler γ function

$$\frac{1}{\Gamma(\alpha)} = \int_\sigma \frac{dz}{2\pi i} e^z z^{-\alpha} = \tag{A.2}$$

We choose the convention for the logarithm discontinuity at the negative part of the real axis (*principal logarithm*).

Therefore we can write more explicity

$$= \lim_{\epsilon\to 0} \int_{-\infty-i\epsilon}^{i\epsilon} \frac{dz}{2\pi i} \frac{e^z}{e^{\alpha(\ln|z|+i\arg z)}} + \int_{i\epsilon}^{-\infty+i\epsilon} \frac{dz}{2\pi i} \frac{e^z}{e^{\alpha(\ln|z|+i\arg z)}} =$$

With the convention chosen, we obtain that $\arg z = -\pi$ and $\arg z = \pi$ respectively in the first and in the second integral. Changing the variable with $t := -z \pm i\epsilon$

and calculating the limit, we obtain

$$= \int_0^{+\infty} \frac{dy}{2\pi i} \frac{e^{-y}}{y^\alpha} \left(e^{i\alpha\pi} - e^{-i\alpha\pi}\right) = \frac{\sin(\alpha\pi)}{\pi} \int_0^{+\infty} dy\, e^{-y} y^{-\alpha} =$$

In the last term we can recognise the definition of Euler's Γ function, and in the end the expression becomes

$$= \frac{\sin(\alpha\pi)}{\pi} \Gamma(1-\alpha) = \frac{1}{\Gamma(\alpha)}$$

where the last equal sign is due to Euler's reflection formula, which is valid if $\alpha \notin \mathbb{Z}$. In the present case $\alpha = \frac{n}{2}$ where n is an odd integer, so no domain problems arise.

A.3 The integral of $\frac{\cos(\alpha t)}{\cosh^2(t)}$

In the calculations above we encountered an integral of the form

$$I(\alpha) = \int_{-\infty}^{+\infty} dt \frac{\cos(\alpha t)}{\cosh^2(t)} \tag{A.3}$$

which can be also calculated thanks to the residue theorem. We can write the integral above as the limit for $M \to \infty$ of the integral along the segment $[-M, M]$ on the real axe, allowing the variable t to take also complex values.

We close this segment creating a rectangle of vertices $-M$, M, $M+i\pi$, $-M+i\pi$. This path sorrounds the $t = i\pi/2$ second order pole due to the denominator. The integrals along the vertical segments vanish in the $M \to \infty$ limit because the numerator of the integrand is a limited quantity meanwhile the denominator diverges.

So we obtain

$$\lim_{M\to\infty} I_M(\alpha) + \int_M^{-M} dt \frac{\cos(\alpha(t+i\pi))}{\cosh^2(t+i\pi)} = 2\pi i \mathrm{Res}\left(\frac{\cos(\alpha t)}{\cosh^2(t)}, \frac{i\pi}{2}\right) =$$

In the second addend of the first term of the equation above, we can recognise $-\cosh(\alpha\pi) I_M(\alpha)$ and the residue can be calculated as follows

$$= 2\pi i \lim_{t\to i\pi/2} \frac{d}{dt} \left(\left(t - \frac{i\pi}{2}\right)^2 \frac{\cos(\alpha t)}{\cosh^2(t)} \right) = -2\pi\alpha \sinh\left(\alpha\frac{\pi}{2}\right)$$

which becomes the value above after some algebra.

In the end it results

$$I(\alpha) = \frac{-2\pi\alpha \sinh\left(\alpha\frac{\pi}{2}\right)}{1 - \cosh(\alpha\pi)} = \frac{\pi\alpha}{\sinh\left(\alpha\frac{\pi}{2}\right)}$$

Appendix B

The free electron gas

B.1 2D calculations

In this appendix we aim to calculate the grand partition function Ω_0 of a 2D free electron gas at $T = 0$ using Peierls' method. So the single particle energy is $\epsilon = \frac{\hbar^2 k^2}{2m^*}$ and the canonical partition function is $Z(\beta) = g_s \sum_{k_x k_y} e^{-\beta \epsilon_{k_x k_y}}$, where $g_s = 2$ is the spin degeneracy of each electron.

The electrons are confined in $L \times L$ box, so imposing the period boundary conditions we obtain $k_j = \frac{2\pi n_j}{L}$ where $j = x, y$ and $n_j \in \mathbb{Z}$. The number of states in the annulus $2\pi k dk$ is $2\frac{2\pi k dk}{\left(\frac{2\pi}{L}\right)^2}$, so the density of states per unit area in k space is $\rho(k) = \frac{Ak}{\pi}$ and the denisty of states as a function of the energy is $\rho(\epsilon) = \rho(k)\frac{dk}{d\epsilon} = \frac{Am^*}{\pi\hbar^2}$.

To calculate the partition function, we take the limit to the continuum and we change to polar coordinates in the k space, so that we can write the sum as the integral

$$Z(\beta) = \frac{A}{2\pi^2}\int_0^{+\infty} dk\, 2\pi k e^{-\beta\frac{\hbar^2 k^2}{2m^*}} = \frac{Am^*}{\pi\hbar^2\beta} \tag{B.1}$$

In the limit of low temperature, as already explained, we can derive $\Omega_0 = -B(\mu)$, where

$$B(\epsilon) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{s\epsilon}\frac{Z(s)}{s^2} = \frac{Am^*}{\pi\hbar^2}\int_{c-i\infty}^{c+i\infty}\frac{ds}{2\pi i}\frac{e^{s\epsilon}}{s^3}$$

As done in the $H \neq 0$ case, we can write the integral above I_0 as a part of the integral along the path in figure 7.2. Here there is only one third order pole $s = 0$ inside the path, so we can simply calculate its residue from the Laurent expansion $\frac{e^{s\epsilon}}{s^3} = \frac{1}{s^3} + \frac{\epsilon}{s^2} + \frac{\epsilon^2}{2s} + O(1)$ which leads to $I_0 = \frac{\epsilon^2}{2}$ and in the end we obtain

$$\Omega_0 = -\frac{Am^*}{2\pi\hbar^2}\mu^2 \tag{B.2}$$

B.2 3D calculations

In this appendix we aim to calculate the grand partition function Ω_0 of a 3D free electron gas at $T = 0$ using Peierls' method. So the single particle energy is $\epsilon = \frac{\hbar^2 k^2}{2m^*}$

and the canonical partition function is $Z(\beta) = g_s \sum_{k_x k_y k_z} e^{-\beta \epsilon_{k_x k_y k_z}}$, where $g_s = 2$ is the spin degeneracy of each electron.

The electrons are confined in $L \times L \times L$ box, so imposing the period boundary conditions we obtain $k_j = \frac{2\pi n_j}{L}$ where $j = x, y, z$ and $n_j \in \mathbb{Z}$. The number of states in the spherical shell $4\pi k^2 dk$ is $2\frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3}$, so the density of states per unit volume in k space is $\rho(k) = \frac{Vk^2}{\pi^2}$ and the denisty of states as a function of the energy is $\rho(E) = \rho(k)\frac{dk}{dE} = \frac{\sqrt{2}V(m^*)^{3/2}\sqrt{E}}{\pi^2\hbar^3}$.

To calculate the partition function, we take the limit to the continuum and we change to spherical coordinates in the k space, so that we can write the sum as the integral

$$Z(\beta) = \frac{V}{\pi^2}\int_0^{+\infty} dk\, k^2 e^{-\beta\frac{\hbar^2 k^2}{2m^*}} = 2V\left(\frac{m^*}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} \tag{B.3}$$

In the limit of low temperature, as already explained, we can derive $\Omega_0 = -B(\mu)$ where

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

As done in the $H \neq 0$ case, we can write the integral above I_0 as a part of the integral along the path in figure 7.3. Here there are no poles inside the path so we can simply calculate

$$I_0 = \int_\sigma \frac{ds}{2\pi i}\frac{e^{s\epsilon}}{s^{7/2}} = \frac{\epsilon^{5/2}}{\Gamma\left(\frac{7}{2}\right)}$$

In the end we obtain

$$\Omega_0 = -B(\mu) = -\frac{16}{15\sqrt{\pi}}V\left(\frac{m^*}{2\pi\hbar^2}\right)^{\frac{3}{2}}\mu^{5/2} \tag{B.4}$$

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