

The De Haas - Van Alphen Effect
in Layered Conductors

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by

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Abstract

The de Haas - van Alphen effect method is used to analyze organic layered conductors. The oscillatory part of the magnetization and its period of oscillation are explicitly expressed in terms of the Fermi surface parameters for possible quadratic form of quasitwodimensional energy spectrum. The Fermi liquid theory is also used to examine the results and it is found to influence slightly the amplitude and period of oscillation.

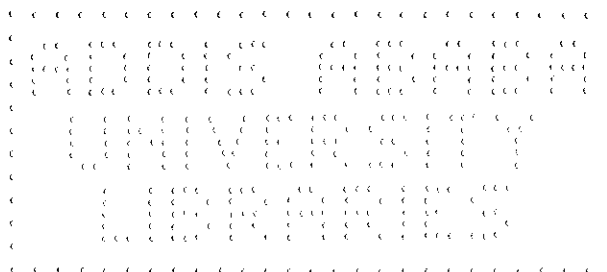
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Introduction

This thesis is devoted to the theoretical analysis of the de Haas -van Alphen effect in layered conductors, which have quasi-two-dimensional energy spectra of charge carriers.

There is a class of measurable quantities valued primarily because they contain detailed information about the geometric structure of the Fermi surface. Such quantities depend only on universal constants, experimentally controlled variables (such as temperature, frequency, magnetic field strength, crystal orientation) and information about the electronic band structure that is entirely determined by the shape of the Fermi surface. But informations about the shape of the Fermi surface which may also involve a series of experiments are vital in the determination of transport coefficients. Quantities yielding such Fermi surface information have significant importance in the physics of metals, and their measurement almost always requires single crystals of very pure substances at very low temperatures and is frequently performed in very strong magnetic fields (for example, de Haas-van Alphen effect) or in high frequency electromagnetic fields (Anomalous Skin Effect). These effects are based on the same underlying physical mechanism, and their techniques appear to be powerful and simple. There is no doubt that this method can also be applied to layered conductors.

The significant part of these conducting materials have layered structures, the electric conductivity of which under normal (non superconducting) condition along the layers considerably exceeds electric conductivity along the direction normal to these layers. For verifying the mechanism of formation of superconducting condition, it is important to

know the properties of the elementary excitations, which are responsible for the transposition of electrical charges in the crystal. The observation of the de Haas - van Alphen and the Shubnikov - de Haas effects in layered organic conductors makes justified the supposition that the system of fermions which is similar to conduction electron in metals but possessing quasi-two-dimensional energy spectrum is responsible for their electron properties. Consideration of the high frequency electromagnetic wave encourages one to consider the Fermi liquid theory in the results.

It is not difficult to judge the significance of the knowledge of the Fermi-surfaces of these layered conductors in the progress of some more demanded technologies which can entail further fascinating researches via their important properties such as electrical and thermal conductivity and etc. The intensive development of microelectronic engineering and computing facilities defines constant exploration of new conducting junctions which can be described through the analysis of these conductors and possessing properties considerably differing from the properties of usual metals and semiconductors. In the meantime, the study of these artificially synthesized conductors generally having complicated compositions and structure serves as a source of new and frequently unique information about the fundamental processes in solids.

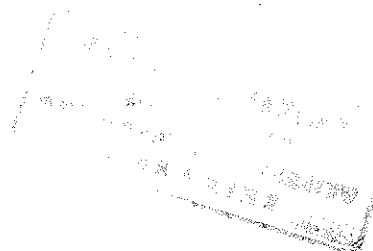
There is relatively large group of organic conductors possessing metallic type of temperature dependence of conductivity and layered structure, the electric conductivity of which under normal (non superconducting) condition along the layers considerably exceeding electric conductivity along the direction normal to these layers. Among these are tetratriafulvaline salt $(BEDT-TTF)_2X$ (where $X = I_3, IBr_2, AuI_2, NH_4Hg (SeCN)_4, KHg$

(SeCN)₄, Cu (NCS)₂, RbHg (SeCN)₄, TlHg (CSN)₄ and halogens of tetraselentetracen (TSeT)₂Cl are examples of such conductors. These conductors usually are called organic metals [1], underlining thus their relationship with usual metals and relatively large life time of their elementary excitations which carry the charges e with energy close to the Fermi energy. By present time, a series of methods are already offered to layered organic conductors, which were applied to normal metals earlier.

The observation of the de Haas - van Alphen and the Shubnikov - de Haas effects in layered organic conductors makes justified the supposition that the system of fermions which is similar to conduction electron in metals but possessing quasi-two-dimensional energy spectrum is responsible for their electronic properties[1].

The thesis is divided into three chapters. In the first chapter is a short and general preview covering some topics, essential in answering questions which may arise in relation to the discussions put in the main topic in chapter 3, such as the theory of electrons in a periodic crystal lattice, some important ideas of energy spectrum (including tight - binding and nearly - free electron approximations and then energy spectrum in our layered conductors), the quasi particle concept as applied to the Fermi liquid theory and then the resulting transport equation, some ideas of motion of an electron in a uniform magnetic field which is important in the discussion about semiclassical quantization of energy levels

In the second chapter, the general theory of electrons in a magnetic field is formulated through the discussions on Pauli - paramagnetism and Landau - diamagnetism, semiclassical quantization of energy levels for an arbitrary electronic system is discussed and then applied to layered conductors.



Chapter 3 is devoted to an exposition of the de Haas van Alphen effect. The general expression for the thermodynamic potential and from that the oscillatory part of the magnetization is derived using simple method. Then this general result, which is valid for arbitrary form of energy spectrum, is applied to layered conductors in which explicit expressions for the oscillatory term in the magnetization and the periods of oscillations are stated for particularly simple quadratic form of our layered conductor energy spectrum. A theoretical plot showing the oscillation is also displayed for this simple case and it is found to be similar to experimental plot for Bismuth. Of the factors affecting the nature of this oscillation, the Fermi - liquid effect is discussed. It is found that there is a slight modification of the amplitude and period of the oscillation due to the consideration of this effect. But, as mentioned in chapter one, it does not change the result qualitatively.

Overall conclusion is given in the conclusion part of the thesis, whereas the used monographs and original sources used in formulation of the thesis are listed in Reference.

Chapter 1

General Properties of Electrons in Metal (Preview)

1.1 Electrons in a Periodic Crystal Lattice

The free electron theory is based up on the notion that the conduction electrons within a metallic substance act like the classical free particles of a gas, subject only to the limitations of the Fermi-Dirac statistics [2]. The fact that metals are good conductors of heat and electricity is due to the considerable overlap between electron states belonging to the outer shells of the constituent atoms. As a result, these so-called valence electrons move easily from one atom to the next, so that one cannot even say to which atom they really belong. In view of the small overlap between inner shell states, they can be assumed to be essentially the same as in isolated atoms and termed free or conduction electrons. Thus, a metal can be thought of as a “sea” of valence electrons moving in a crystalline lattice of ions. These electrons interact quite strongly among themselves and with the ions, the potential energy of interaction being comparable in fact to the electronic kinetic energy. Depending on the situations at hand, these electrons may be categorized as electron fluid and electron gas [3].

A strongly interacting system of electrons constitute electron fluid. And a system of non-interacting electrons in an external field, consisting of the average field of the ions and of the other electrons, constitute electron gas. The concept of electron fluid will be clear when we come to section 1.6; and we try to see here some important aspects of electron

gas in periodic lattice, usually known as Bloch - electrons, since many conclusions can be drawn from the symmetry of such a lattice even though the theory of periodic lattice may seem oversimplified.

Generally, the one electron wave function for a perfectly periodic potential $V(\mathbf{r})$, is the solution to Schrodinger's equation and is given by

$$\psi(\mathbf{r}) = e^{i\mathbf{p}\mathbf{r}/\hbar}u(\mathbf{r}). \quad (1.1)$$

The potential $V(\mathbf{r})$ is periodic in \mathbf{r} with a periodicity of the lattice vector given by $\mathbf{a}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$. Where each n_i ($i = 1, 2, 3$) is an integer running over positive and negative values as well as zero, and each \mathbf{a}_i is primitive translation vector; so that $V(\mathbf{r}) = V(\mathbf{r} + \mathbf{a}_n)$. The function $u(\mathbf{r})$ is also periodic in \mathbf{r} with the same periodicity as $V(\mathbf{r})$, i.e., $u(\mathbf{r}) = u(\mathbf{r} + \mathbf{a}_n)$ and is known as Bloch function. Equation (1.1) is known as Bloch's theorem [2, 3]. The wave function $\psi(\mathbf{r})$ is like a plane wave $e^{i\mathbf{p}\mathbf{r}/\hbar}$ describing the motion of a free particle, but is modulated by a periodic function $u(\mathbf{r})$, due to the presence of the periodic potential $V(\mathbf{r})$. As a result the vector \mathbf{p} , which is analogous to the momentum of a free particle, is not the actual momentum of the particle in the usual sense of that term. It is called the crystal momentum of the electron.

It is clear that the energy of the electron depends on the vector \mathbf{p} . Since \mathbf{p} and $\mathbf{p} + \hbar\mathbf{K}$ are physically equivalent, the energy $\varepsilon(\mathbf{p})$ must be a periodic function of \mathbf{p} with periods $\hbar\mathbf{K}$, where \mathbf{K} is reciprocal lattice vector. So that several energy levels $\varepsilon_l(\mathbf{p})$ can exist for a given \mathbf{p} , with each of these functions $\varepsilon_l(\mathbf{p})$ has a periodicity of $\hbar\mathbf{K}$.

Since the vectors \mathbf{p} and $\mathbf{p} + \hbar\mathbf{K}$ are physically equivalent, it is sufficient to consider only a single primitive unit cell in the reciprocal space. The volume of such a domain

where \mathbf{p} is uniquely defined is $\frac{(2\pi\hbar)^3}{v}$, with $v = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ being the volume of a primitive unit cell of the crystal lattice.

However, successive levels will be infinitesimally close to each other in a very large volume. We shall actually be interested only in the density of states, i.e., in the number of states per unit volume in reciprocal space.

Consider a parallelepiped sample of dimensions L_1, L_2, L_3 . Imposing periodic boundary conditions at the ends of the sample, we get that \mathbf{p} is a discrete variable with components $p_i = \frac{2\pi\hbar n_i}{L_i}$, so that the density of states for each spin orientation is given by [3]

$$\nu(\mathbf{p}) = \frac{v}{(2\pi\hbar)^3}. \quad (1.2)$$

It is also important to take into account the fact that there are two components $s_z = \pm\frac{1}{2}$ of spin along a given direction for a given value of \mathbf{p} . This results in doubling the number of levels. As a result a total of $2N$ levels is associated with each function $\varepsilon_l(\mathbf{p})$. The functions $\varepsilon_l(\mathbf{p})$ are periodic in reciprocal space and, hence, oscillate between certain maximum and minimum values. For every l we, therefore, obtain a band of allowed energy values. These bands may be separated by energy gaps, i.e., energies which no electron can have, but can also overlap.

From the invariance of the full Schrodinger equation under the transformation $t \rightarrow -t$ and $\psi \rightarrow \psi^*$ follows that, the energy bands $\varepsilon_l(-\mathbf{p})$ and $\varepsilon_l(\mathbf{p})$ are equal.

The primitive unit cell of the reciprocal lattice is chosen as the natural domain in which \mathbf{p} is uniquely defined. However, more convenient definition is possible. This new domain of definition for \mathbf{p} is called the Brillouin zone defined by conditions defining this

zone namely [3]

$$|\mathbf{p}\mathbf{a}_i| = |p_i a_i| \leq \pi \hbar, \quad (1.3)$$

which hold for every basis vector \mathbf{a}_i . One-dimensional Brillouin zone reduces to the interval $-\frac{\pi\hbar}{a} < p \leq \frac{\pi\hbar}{a}$, where a is the period of the linear chain.

1.2 The Energy Spectrum

1.2.1 The Tight-binding and the Nearly-free Electron Approximations

Accurate calculations of the energy bands $\varepsilon_l(\mathbf{p})$ require rather complex techniques. In order to illustrate the general properties of the energy bands $\varepsilon_l(\mathbf{p})$ obtained above one can consider two simplest approximations [2, 3], although they are not suited for an accurate determination of the energy bands $\varepsilon_l(\mathbf{p})$ of real metals: the tight-binding approximation and the nearly-free electron approximation.

In tight-binding approximation, it is assumed that electronic shells do not overlap appreciably and that each electron can be assigned to a particular atom as a zero-order approximation. Overlap between shells will be considered as a perturbation.

The potential energy of an electron in the field of all the ions has the form $V(x) = \sum_n U(x - na)$, which is only different from zero in the neighborhood of the n^{th} ion. In one dimensional case one sees that $\varepsilon_l(\mathbf{p})$ is a periodic function of \mathbf{p} with period $\frac{2\pi\hbar}{a}$ and has a form (A and B being constants) [3]

$$\varepsilon = A + B \cos(pa/\hbar). \quad (1.4)$$

Calculations are more complicated in three dimensions. In the simplest case, corresponding to one atom per unit cell with a single s electron for a bcc lattice if only nearest-neighbors are taken into account one finds

$$\varepsilon = C + D \cos(p_x a / 2\hbar) \cos(p_y a / 2\hbar) \cos(p_z a / 2\hbar),$$

where D determines the bandwidth.

The physical significance of these results is that the discrete levels of individual atoms broaden into narrow bands whose width depends on the amount of overlap or, more precisely, on the matrix element corresponding to the transfer of an electron to a neighboring atom. The resulting expressions are applicable when the overlap is small, i.e., for the inner shells. Some of the energy bands of transition metals can therefore be determined by means of this method.

In nearly-free electron approximation, we consider the opposite case in which the conduction electrons are nearly free and the crystal potential is weak so that perturbation theory is applicable.

The normalized wave function of a free electron (in one dimension) is $L^{-\frac{1}{2}} e^{i\frac{px}{\hbar}}$, where L is the length of the chain. Its energy is $\varepsilon^{(0)} = \frac{p^2}{2m}$. Such an electron is acted upon by a potential $U(x)$, which can be expanded in a Fourier series in view of its periodicity: $U(x) = \sum_n U_n e^{\frac{2\pi i n x}{a}}$, where $\frac{2\pi n}{a}$ are the periods of the reciprocal lattice in the one-dimensional case. The matrix elements of $U(x)$ between states like $L^{-\frac{1}{2}} e^{i\frac{px}{\hbar}}$ are $U(p, p')$ and are obviously equal to zero unless $p - p' = \frac{2\pi n \hbar}{a}$, in which case $U(p - p') = U_n$. The first order correction to the energy $\varepsilon^{(0)}(p)$ is, therefore, a constant which can be absorbed by redefining the zero of energy.

Noting that perturbation theory is valid if the higher-order correction is small compared with lower one (generally, $U_{n+1} \ll U_n$), we see that $\varepsilon(p)$ exhibits a jump discontinuity equal to $2|U_n|$ at $p = \frac{\pi\hbar}{a}n$.

An electron moving through a lattice must actually be characterized by its crystal momentum. We can go to that representation by subtracting from \mathbf{p} , the period of the reciprocal lattice (times \hbar) corresponding to a particular interval, such that, the difference falls within the Brillouin zone [3, 4]: $U(\mathbf{r}) = \sum_{\mathbf{K}} U_{\mathbf{K}} e^{i\mathbf{K}\mathbf{r}}$.

On going from dependence of energy on crystal momentum, rather than on momentum, we again obtain a general picture of energy bands as [3]

$$\varepsilon(\mathbf{p}) = \frac{1}{2} [\varepsilon^{(0)}(\mathbf{p}) + \varepsilon^{(0)}(\mathbf{p} - \hbar\mathbf{K})] \pm \frac{1}{4} \{ [\varepsilon^{(0)}(\mathbf{p}) - \varepsilon^{(0)}(\mathbf{p} - \hbar\mathbf{K})]^2 + |U_{\mathbf{K}}|^2 \}^{1/2}.$$

Ordinary perturbation theory fails for values of \mathbf{p} such that $\varepsilon^{(0)}(\mathbf{p}) = \frac{p^2}{2M} = \varepsilon^{(0)}(\mathbf{p} - \hbar\mathbf{K})$ or

$$p \cos \theta = \frac{1}{2} \hbar K, \quad (1.5)$$

where θ is the angle between \mathbf{p} and \mathbf{K} . This is the equation of a plane in reciprocal space, perpendicular to the vector \mathbf{K} , and intersecting it at a distance $\frac{1}{2}\hbar K$ from the origin. If \mathbf{K} is the shortest reciprocal vector in a particular direction, this plane is simply a Brillouin-zone boundary. The energy discontinuity occurring on it is one of the reasons why the Brillouin zone is the most convenient domain of definition for crystal momentum.

The appearance of bands in the weak-binding limit has the following physical significance. The condition (1.5) is the condition for Bragg reflection of the plane waves, describing the motion of an electron by crystal planes. Whenever that condition is satisfied, a "free" electron moving through the lattice is strongly reflected by the corresponding

crystal planes, and its wave function is appreciably modified. The energy bands obtained in this case must be such that the component of the electronic group velocity normal to a crystal plane is zero.

1.2.2 Layered Conductor

Recent studies on fermi surfaces show that, there are special class of conductors exhibiting high conductivity along the layers than along the normal to the layers; and termed quasi two-dimensional conductors [5, 6].

From the symmetry and the fact that the conductor is layered, one can judge that an electron act as almost free in its motion in $x - y$ plane (i.e., along the layers), but suffers periodic Bloch potential along z -direction (i.e., along the direction normal to the layers) having periodicity of the layer separation a , and the crystal is said to exhibit anisotropy parallel and perpendicular to the layers. That means, an electron acquires different momenta for the same external field in directions normal and parallel to the layers.

The periodic function $\varepsilon(\mathbf{p})$ can be expanded in Fourier series [7]. Decomposing \mathbf{p} into $\mathbf{p}_\perp = (p_x, p_y, 0)$ and $\mathbf{p}_z = (0, 0, p_z)$, we get upon expansion $\varepsilon(\mathbf{p}) = \varepsilon(\mathbf{p}_\perp, p_z) = \sum_n \varepsilon_n(\mathbf{p}_\perp) \exp(i\alpha p_z)$. Where $\varepsilon_n(\mathbf{p}_\perp)$ is the Fourier amplitude constant in \mathbf{p}_z , so that it can only be function of \mathbf{p}_\perp . From the periodicity of ε in \mathbf{p}_z with a periodicity of a reciprocal lattice constant $\mathbf{b} = (0, 0, b)$, i.e., $\varepsilon(\mathbf{p}_\perp, p_z + b\hat{z}) = \varepsilon(\mathbf{p}_\perp, p_z)$, we obtain $\alpha b = 2\pi n$ (with n being integer). Noting also that ε_n are symmetric in interchange of n and $-n$ (i.e., $\varepsilon_{+n} = \varepsilon_{-n}$) this gives us

$$\varepsilon(\mathbf{p}) = \varepsilon_0(p_x, p_y) + \sum_{n=0}^{\infty} 2\varepsilon_n(p_x, p_y) \cos\left(\frac{na p_z}{\hbar}\right). \quad (1.6)$$

The coefficients $\varepsilon_n(p_x, p_y)$ rapidly decrease with increasing n , i.e., $\varepsilon_{n+1}(\mathbf{p}_\perp) \ll \varepsilon_n(\mathbf{p}_\perp)$. Therefore, for larger n 's, one can say that ε_n is weak function and even can be assumed as constant in \mathbf{p}_\perp . Ignoring the second and higher order terms and denoting $2\varepsilon_1(\mathbf{p}_\perp)$ by $\varepsilon_1 =$ constant, we get a less general equation for the energy spectrum of our layered sample to be

$$\varepsilon(\mathbf{p}) = \varepsilon_0(p_x, p_y) + \varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right), \quad (1.7)$$

the most general one being (1.6). Note that we have found the same form of $\varepsilon(\mathbf{p})$ as in (1.4). If $\varepsilon_0(p_x, p_y)$ is quadratic in its arguments, the last equation represents the energy spectrum of corrugated cylinder and can be written as [3]:

$$\varepsilon(\mathbf{p}) = \frac{p_x^2 + p_y^2}{2m} + \varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right). \quad (1.8)$$

1.3 The Quasi-particle Concept

1.3.1 The Quasi-particle

In the previous sections, we had been dealing with the behavior of a single electron in the average field of the lattice and of the other electrons, but we didn't focus in particular on the nature of the interaction between the electrons apart from the coulomb contribution. But, here and in the following two sections, we shall examine an actual system of interacting electrons by considering the total electron-electron interaction including quantum terms in addition to the classical coulomb energy. Such a system of electrons constitute the so called electron fluid. The behavior of such a system can be understood on the basis of Landau's

ideas on the energy spectrum of condensed quantum systems, and of his own theory of Fermi liquids [3, 8], by taking the vibration of crystal lattice as an illustrative model. The simplest illustration of Landau's general approach is provided by the vibrations of a crystal lattice. It is obvious that one can use the de Broglie's hypothesis to describe the motion of real free particle as plane waves; but here, we shall try to see the converse, i.e., for example describing the elastic waves associated with lattice vibration as a motion of some fictitious particles known as phonons, and thus, generalizing this to other waves, we call them quasiparticles. In addition to phonons, typical examples are photons, which are used to describe the propagation of electromagnetic waves.

In lattice vibrations, if the amplitudes of oscillations are small, the potential energy of interaction between atoms (phonons) in the crystal can be expanded in powers of the atomic displacements up to second order. Noting that all the first order terms vanish, since the equilibrium configuration corresponds to a potential energy minimum, and then solving the corresponding equations of motion, we obtain the displacement of each oscillator (quasi particle known as here phonons). Each of these displacements being $\sim e^{i(\mathbf{k}\mathbf{a}_n - \omega t)}$, serves as the wave function of the elastic wave of wave vector $\mathbf{k} = \mathbf{p}/\hbar$, with \mathbf{p} being the quasi momentum of each phonon. The corresponding eigen values give the energies of a system of coupled oscillators, each with energy levels $\hbar\omega (n + \frac{1}{2})$. This result reminds us the wave function of a free particle given by

$$e^{\frac{i}{\hbar}(\mathbf{p}\mathbf{r} - \varepsilon t)}, \quad (1.9)$$

and appearing as elementary excitation of energy $\zeta(\mathbf{p}) = \frac{\mathbf{p}^2}{2m^*}$. This energy is known as the quasiparticle energy corresponding to a quanta of energy $\hbar\omega$ for a system of the coupled oscillators.

At higher temperature below the melting point of the solid, the amplitude of oscillation may increase beyond the inter atomic distance and the phonon picture may fail. So that one may be forced to take the higher order terms in the expansion of the total potential energy for phonon picture to be valid. But in most real metals, this temperature is beyond the melting point, so that, the corresponding quasi particle representation is valid almost at all temperatures. Thus, one can summarize Landau's [9] idea as follows: any homogeneous system containing a large number of particles has low-lying states similar to those of vibrating lattice, and the properties of such a system can be described in terms of quasi particle model.

Generally, quasi particles can have integer ($n\hbar$) or half integer ($(n + 1/2)\hbar$) spins; i.e., they can be either Bosons or Fermions. The statistics of quasiparticles bear no unique relationships to the statistics of real particles constituting the quasi particle itself. The energy of a quasi particle is a function of its momentum, the corresponding relation $\varepsilon(\mathbf{p})$ is the main characteristics of such low-lying excited states.

Electrons have spin of $(1/2)\hbar$ each, as a result they form a Fermi liquid. According to Landau's hypothesis, the energy spectrum of such a liquid is very similar to that of an ideal Fermi gas.

1.3.2 The Fermi Gas

Let us consider the free electron gas for a start. The equilibrium distribution function is the well-known Fermi function

$$n_0(\varepsilon) = \left(e^{(\varepsilon - \mu)/kT} + 1 \right)^{-1}, \quad (1.10)$$

where ε is the state energy of each qasiparticle and μ is the chemical potential. At $T = 0$, $\varepsilon = \varepsilon_0 = \frac{p^2}{2M}$ and $\mu = \mu(0)$, so that $n_0(\varepsilon)$ is a step function.

The quantity $\mu(0)$ is called the Fermi energy. In terms of the Fermi momentum p_0 , defined so that $\mu(0) = \frac{p_0^2}{2M}$, one finds that at $T = 0$ all states with momenta inside a sphere of radius $p = p_0$ (the Fermi sphere) are occupied, while those outside are unoccupied. This is a consequence of Pauli's principle, that only one particle can be in any given state, so that the lowest states are filled at $T = 0$. We know that in accordance with Pauli's principle, within the volume $\left(\frac{2\pi\hbar}{L}\right)^3$ of momentum-space, there can be 2 states, correspondingly the number N of occupied states (= number of particles, since all states are occupied) in our Fermi sphere of volume $\frac{4\pi}{3}p_0^3$, is determined from $\frac{2}{\left(\frac{2\pi\hbar}{L}\right)^3} = \frac{N}{\frac{4\pi}{3}p_0^3}$ i.e.,

$$N = \frac{2V}{(2\pi\hbar)^3} \frac{4\pi}{3} p_0^3 \text{ or } p_0 = \hbar \left(\frac{3\pi^2 N}{V} \right)^{1/3}. \quad (1.11)$$

Let us consider the case $T \neq 0$. The distribution function is now represented not by the step function. The width of the transition region from the step function is of the order of kT (k being Boltzmann's constant). This reflects the excitation of some particles that are outside the Fermi sphere, having gained an energy of order kT . The equilibrium state at $T \neq 0$, as well as any excited state, can be constructed from the $T = 0$ equilibrium state by transferring particles from inside to outside the Fermi sphere [8]. In each transfer a particle

appears outside the Fermi sphere while an empty state or an “antiparticle” is created inside. These particles and anti-particles are the quasi particles describing excited states of our system. Their energies must be measured from the Fermi level $\mu(0) = \frac{p_0^2}{2m}$. If $p - p_0 \ll p_0$, particle-like quasi particles with momenta exceeding p_0 have energy

$$\xi_p(p) \cong v(p - p_0), \quad (1.12)$$

with $v = \frac{pF}{M}$ being the velocity on the Fermi sphere. Antiparticles, on the other hand, have momenta below, p_0 and their energies are measured in the opposite direction, i.e., $\xi_a(p) \cong v(p_0 - p)$.

1.3.1 Quasiparticles in an Isotropic Fermi Liquid

According to the hypothesis, the quasi-particle spectrum of an isotropic Fermi liquid of strongly interacting identical particles is similar to that of the ideal gas. This means that there is a certain value p_0 which, according to Landau’s theory [3, 9], is still related to the particle density by the ideal gas formula (1.11). Two kinds of quasi particles exist: particle-like with $p > p_0$, and antiparticle-like with $p < p_0$. So long as $|p - p_0| \ll p_0$, their energies are given by $\xi_p(p) \simeq v(p - p_0)$, $\xi_a(p) \simeq v(p_0 - p)$. In the general case, v is an unknown constant having the dimension of velocity. Instead of v one can introduce another constant via the relation $v = p_0/m^*$. The quantity m^* has the dimension of mass, and is called the “effective mass”.

The quasi-particle concept is valid if the damping coefficient $\gamma \ll \xi$, i.e., close to the Fermi level. If one deals with a Fermi liquid in equilibrium at $T \neq 0$, the relevant quasi particles all have energies $\xi \sim T$. The damping coefficient is then of the order $(kT)^2 / \mu$

The description of the liquid in terms of quasi particles is therefore valid only so long as [3] $kT \ll \mu$.

For electrons in metals the quantity \hbar/p_0 (the de Broglie wavelength) is of the same order as interatomic distances, i.e., 10^{-8} cm, so that $p_0 \sim 10^{-19}$ g cm s⁻¹. Therefore, one obtains $T \ll T_0 \sim (10^4 - 10^5)$ K. This condition shows that the quasi-particle picture certainly applies to solid metals at all temperatures, since T_0 significantly exceeds the melting temperature in any case.

1.3.3 The Anisotropic Fermi Liquid

In order to understand the main features of the spectra of electrons in metals, let us first "switch off" the interaction between electrons or, rather, let us consider a gas of non interacting electrons placed in an average periodic field. The states of a single particle in such a field were analyzed in section 1.1. As shown there, the energy levels form bands separated by forbidden gaps. Each band contains $2N$ states, where N is the number of unit cells in the sample [2, 3].

If the Fermi level coincides with the upper edge of a band, some bands are then completely filled, whereas others are completely empty. In such a case a sufficiently weak electric field cannot give rise to a net current, and the substance will be an insulator rather than a metal. If the Fermi level falls within the center of a band the band is called a conduction band. An arbitrarily weak electric field can give rise to current flow. This situation describes a metal. Semiconductors belong to the first category, but the gap between occupied and unoccupied states is then small. Their properties are, therefore, similar to those of

metals unless the temperature is very low [10]. We shall limit our attention to actual metals, however.

The position of the Fermi level for the electron gas in a crystal is fixed by the condition $\varepsilon(\mathbf{p}) = \mu$. This equation describes a surface in momentum space called the Fermi surface. Its symmetry is determined by that of the lattice. In this case, it is also possible to define "particle-like" and "antiparticle-like" quasi particles with momenta outside and inside the Fermi surface, respectively.

In general, the Fermi surface may have a very complex shape. It has a very simple shape in two cases, however [4, 11, 12]. The first one corresponds to an almost empty band. Only a few electrons are present, and, at $T = 0$, they fill up the lowest available states, and must all be in the vicinity of the minimum of $\varepsilon(\mathbf{p})$. If this minimum occurs at $\mathbf{p}^{(0)}$, we may expand the energy in powers of $(\mathbf{p} - \mathbf{p}^{(0)})$. For a cubic crystal with $\mathbf{p}^{(0)} = 0$ one obtains

$$\varepsilon(\mathbf{p}) = \varepsilon_0 + \frac{\mathbf{p}^2}{2m^*}, \quad (1.13)$$

where m^* is a constant called the band effective mass. In the more general case of arbitrary symmetry, but with $\mathbf{p}^{(0)} = 0$ as before, one obtains a positive definite quadratic form instead of \mathbf{p}^2 . After a principal axis transformation it has the form

$$\varepsilon(\mathbf{p}) = \varepsilon_0 + \frac{1}{2} \left(\frac{p_x^2}{m_1} + \frac{p_y^2}{m_2} + \frac{p_z^2}{m_3} \right).$$

A similar situation occurs in the case of an almost filled band. One can then deal with "holes", i.e., empty states in the band, rather than electrons. They will all occur near energy maxima. In the case of a cubic crystal with $\mathbf{p}^{(0)} = 0$ one has $\varepsilon(\mathbf{p}) = \varepsilon_0 - \frac{\mathbf{p}^2}{2m^*}$. This means that holes behave as particles with a negative mass. Generalizations for arbitrary symmetry

and $p^{(0)} \neq 0$ are trivial: In all cases just considered, the Fermi surface is an ellipsoid or consists of a set of ellipsoids.

If the number of electrons per unit cell is odd, some bands may be completely filled, but, as pointed out earlier, at least one band will only be partly filled. If there is only one such band, it must contain N electrons. Since the whole Brillouin zone contains $2N$ states, the volume inside the volume enclosed by the Fermi surface and the Brillouin zone faces (if the former makes contact with these faces) must be half that of the Brillouin zone. The substance is then metal. If the number of electrons per unit cell is even it does not mean the substance is necessarily an insulator. In order to have small numbers of electrons and holes, both an even number of electrons per unit cell and a small overlap between the highest two relevant bands are required. If this is the case, some of the electrons from the highest occupied band (the so-called valence band) will spill over into the lowest unoccupied band (the conduction band), so that it will contain a small number of electrons, while the other band will contain an equal number of holes. This situation occurs in the "semimetals". In addition, a metal might have several partly filled bands, one of which contains a small number of electrons or holes.

The non interacting gas model actually describes the properties of quasi particles in a real metal just as a free-electron gas can be used to describe the quasi-particle properties of an isotropic Fermi liquid. In this context, it is important to remember that the only relevant properties of the gas model are those involving particles close to the Fermi surface. As a result, our previous discussion referring to electrons "filling" bands may seem of doubtful validity, since "deep" states were certainly involved in those arguments.

1.4 Static Transport Coefficients

1.4.1 The Electron as a Wave Packet

Up to now we described electrons by means of stationary solutions of the Schrodinger equation of the Bloch type, $\Psi = e^{i\mathbf{p}\mathbf{r}/\hbar}u(\mathbf{r})$. These functions are not suited for studying transport phenomena, since they correspond to a well-defined value of the crystal momentum \mathbf{p} while the position coordinate remains completely undetermined. This defect can be remedied by constructing a wave packet from Bloch states [3]. One would nevertheless like to retain a reasonably sharply defined crystal momentum. We shall therefore take a superposition of Bloch states with a small spread $\Delta\mathbf{p}$. The width of this interval is restricted by the maximum allowed uncertainty in position. According to the uncertainty principle, one has $\Delta p \Delta r \sim \hbar$.

Since in the last section we had stressed that for the validity of quasi particle representation, the temperature is such that the maximum displacement of each quasi particle (the amplitude of vibration) must be less than the inter atomic distance a , the fact that the maximum uncertainty in position is the displacement of the particle itself confirms us that $a \gg \Delta r$. But, being scattered as a wave, an electron has a finite mean free path $l \gg a$. Therefore, the uncertainty in position must be smaller than l . Also the maximum allowed value of Δp is clearly the momentum of the particle itself. Hence, the restriction $p \gg \Delta p \sim \hbar/\Delta r \gg \hbar/l$ must therefore be obeyed for the wave packet description to make sense.

Another restriction for the validity of the quasi particle representation is that the quasi particle energy ξ is such that $\xi = \varepsilon - \mu \gg \gamma$ where γ is the damping coefficient, which

appears in the wave function of a quasi particle $\exp(i\xi t/\hbar - \gamma t/\hbar)$. The coefficient γ is related to the mean lifetime τ , e.g., $\gamma \sim \hbar/\tau$. And since $\xi \sim kT$ for a Fermi liquid in equilibrium at temperature $T \neq 0$, The second restriction can therefore be written as $\xi \gg \hbar/\tau$ or $kT \gg \hbar/\tau$. Thus the wave packet description is valid under the conditions related to the damping of quasi particles [3] if

$$p \gg \hbar/l \text{ and } kT \gg \hbar/\tau. \quad (1.14)$$

The velocity of an electron described by a wave packet is called the group velocity. It is given by

$$\mathbf{v} = \partial\varepsilon/\partial\mathbf{p}. \quad (1.15)$$

Let us assume that an electron is moving under the influence of an external electric field \mathbf{E} . The work done by the applied field per unit time is $e\mathbf{E}\mathbf{v}$. It must be equal to the energy gained by the electron per unit time. Thus $e\mathbf{E}\partial\varepsilon/\partial\mathbf{p} = \partial\varepsilon/\partial\mathbf{p} \frac{d\mathbf{p}}{dt}$ or

$$\frac{d\mathbf{p}}{dt} = e\mathbf{E}. \quad (1.16)$$

An increasing \mathbf{p} , however, does not necessarily imply that the electron is accelerating. In practice, because of scattering, the momentum of the electron cannot undergo a large change under the influence of the external field. The electron is only accelerated over a mean free path, while the fields that can be set up in metals are never strong enough to effect an appreciable change in electron crystal momentum over a relaxation time. As a result, the electrons effectively remain close to the Fermi surface.

1.4.2 The Boltzmann Kinetic Equation

The wave packet description, valid under the conditions (1.14), enables one to treat electrons as classical particles with simultaneously well-defined values of position and crystal momentum. Let us introduce the distribution function $f(\mathbf{p}, \mathbf{r}, t)$ in phase space. The total time rate of change of f is expressed through its total derivative df/dt . This change is due to collisions of the electron with other electrons, as well as to scattering off defects in the crystal (impurities or structural defects).

We can therefore write

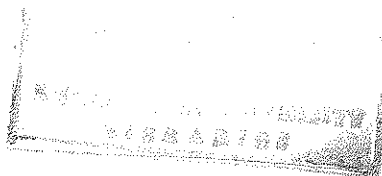
$$\frac{df}{dt} = I(f),$$

where $I(f)$ is the so-called collision integral. This equation is called the Boltzmann kinetic equation. It will be used below to analyze transport phenomena in metals. Expanding the total derivative we obtain the Boltzmann kinetic equation, which accounts for the effects of external fields, gradient in temperature and concentration as

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{r}} + \mathbf{F}_{ex} \frac{\partial f}{\partial \mathbf{p}} = I(f), \quad (1.17)$$

where $\mathbf{v} = \frac{d\mathbf{r}}{dt}$, $\mathbf{F}_{ex} = \frac{d\mathbf{p}}{dt}$ are the velocity and the force on the quasi particle (electron) due to the external fields.

For scattering by impurities (or point defects), using the Born approximation and treating the impurity potential as if it were weak, along with the assumptions that the scattering of electrons is isotropic and elastic, one can obtain simple estimate or illustrate particular calculations. The first assumption is a poor one in real metals, since it holds true only in spherical Fermi surfaces, whereas the second one is not valid for all scattering pro-



cesses. In this approximation (the τ -approximation), it can be shown that $I(f) = -\frac{(f-f_0)}{\tau}$ and one gets for the kinetic equation (1.17)

$$\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{r}} + \mathbf{F}_{ex} \frac{\partial f}{\partial \mathbf{p}} = -\frac{f_1}{\tau};$$

with $f = f_0 + f_1$, such that $|f_1| \ll f_0$, f_0 being the equilibrium distribution function and f_1 is a small variation from the equilibrium one due to the external fields or the gradients and τ is the mean free time between successive collisions [3].

1.5 Motion of an Electron in a Uniform Magnetic field

In this section, we ignore all quantum effects (to be discussed in Chap 3), so that, the force on the quasi particle in presence of the static magnetic field $\mathbf{H} = (0, 0, H)$ is

$$\frac{d\mathbf{p}}{dt} = -\frac{e}{c} \frac{\partial \varepsilon}{\partial \mathbf{p}} \times \mathbf{H} = -\frac{e}{c} \mathbf{v} \times \mathbf{H}. \quad (1.18)$$

The electron undergoes classical motion described by this equation of motion. This motion is along a defined trajectory and in the plane perpendicular to \mathbf{H} , i.e., the plane $p_z = \text{constant}$.

The rate of change of energy is $\frac{d\varepsilon}{dt} = \frac{\partial \varepsilon}{\partial \mathbf{p}} \frac{d\mathbf{p}}{dt} = \frac{\partial \varepsilon}{\partial \mathbf{p}} \left(-\frac{e}{c} \frac{\partial \varepsilon}{\partial \mathbf{p}} \times \mathbf{H} \right) = 0$, and according to (1.18), $\frac{dp_z}{dt}$ is also zero, so that ε and p_z are constants. Hence, the orbit of the quasi particle when moving along closed orbit is determined by the intersection of surfaces $\varepsilon = \mu = \text{const}$ (known as Fermi surface), and $p_z = \text{const}$. If the Fermi surface is closed, all such orbits are closed, but if it is open, the orbit is either open or closed depending on the relative orientation of the magnetic field with the surface.

Let us write (1.18) in component form:

$$dp_x/dt = \frac{e}{c}(v_y H), \quad dp_y/dt = -\frac{e}{c}(v_x H).$$

Squaring and summing the result, one obtains $\frac{dp_x^2 + dp_y^2}{dt^2} = \frac{e^2}{c^2} (v_x^2 + v_y^2) H^2$. Since $\sqrt{dp_x^2 + dp_y^2} = dl$ is the element of length along an electronic orbit in momentum space, $dl/dt = \frac{e}{c} v_{\perp} H$, $v_{\perp} = \sqrt{v_x^2 + v_y^2}$ or, equivalently

$$t = \frac{c}{eH} \int \frac{dl}{v_{\perp}}. \quad (1.19)$$

If the electron's orbit is closed, this integral can be taken around the orbit; the result will obviously be the period of the motion

$$T = \frac{c}{eH} \oint \frac{dl}{v_{\perp}}. \quad (1.20)$$

Consider a plane $p_z = \text{const}$. The enclosed cross-sectional area is given by the integral $S = \int dp_x dp_y$. Instead of evaluating it directly, we can consider the contours $\varepsilon = \text{const}$ in the plane $p_z = \text{const}$ and integrate first along these curves and then along their normals. The width of the ring formed by two such contours, whose energies differ by $d\varepsilon$ is locally equal to $\frac{d\varepsilon}{|\partial\varepsilon/\partial\mathbf{p}|} = \frac{d\varepsilon}{v_{\perp}}$.

The area of this ring is $d\varepsilon \oint \frac{dl}{v_{\perp}}$ (the integral is taken once around the whole contour), and the enclosed area in the plane $p_z = \text{constant}$ is given by

$$S = \int d\varepsilon \oint \frac{dl}{v_{\perp}}.$$

Comparing with (1.20), we find

$$T = \frac{c}{eH} \frac{\partial S}{\partial \varepsilon}. \quad (1.21)$$

Introducing the so-called "cyclotron mass" $m^* = \frac{1}{2\pi} \frac{\partial S}{\partial \varepsilon}$, the period can then be written as

$T = \frac{2\pi c}{eH} m^*$. Let $t_H = \frac{c}{eH} \int_l \frac{dl}{v_{\perp}}$ be the time measured along the orbit as defined above,

then the defining equations (1.19) for t_H have the following solutions: $v_x = v_{\perp} \cos \omega_c t_H$, $v_y = -v_{\perp} \sin \omega_c t_H$; where $\omega_c = eH/m^*c$ is frequency of the motion.

Since in presence of a static magnetic field \mathbf{H} , the quasi-momentum \mathbf{p} of an electron is replaced by the canonical momentum \mathbf{P} conjugate to the canonical coordinate \mathbf{r} , which is given by $\mathbf{P} = \mathbf{p} - \frac{e}{c}\mathbf{A}$ (to be discussed in chapter 2); and since \mathbf{H} , and hence the vector potential \mathbf{A} are constants in time, from (1.18), $\frac{d\mathbf{P}}{dt} = -\frac{e}{c}\frac{d\mathbf{r}}{dt} \times \mathbf{H}$. Upon integrating with respect to t and choosing the constant of integration to be zero, so that the origin of the position coordinate \mathbf{r} and of the corresponding canonical momentum \mathbf{P} conjugate to \mathbf{r} coincide; we get $P_x = -\frac{e}{c}Hy$, $P_y = \frac{e}{c}Hx$ and $P_z = \text{constant}$ [13]. Therefore, one can conclude that the positive P_x -axis coincides with the negative y -axis, the positive P_y -axis with the positive x -axis and positive P_z -axis coincides with the positive z -axis. This enables one to write the trajectory of the electron in the real space.

1.6 The Fermi Liquid Effect

1.6.1 Interaction between Quasiparticles

When we discussed the correspondence between Fermi liquid and an ideal Fermi gas, we deliberately ignored an important complication. Whereas the energy spectrum (1.12) of a Fermi gas is completely determined by the energy of a single free particle, the interaction between quasiparticles, which is by no means weak in general, does play an important role in a real Fermi liquid.

As discussed above, one supposition in Landau theory is that weak excited states of liquids can be described in terms of quasiparticles, which as well as real electrons, have defined momentum and spin, are subject to the Fermi statistics and their number coincides with the number of particles in the liquid. The second supposition is that the interaction of electrons can be described with the help of self-consistent field of the enclosed particles and is explained in that the energy of the system is a functional of the distribution functions of the quasiparticles. In this situation the energy of the quasiparticles, ϵ , is defined as the variational derivative of the total energy relative to the quasi-particle distribution function [8].

Actually, as we shall show in this chapter, the complication does not in general introduce any significant modifications. In most cases it has no effect whatsoever. In other cases it does not change the order of magnitude of previous results. Sometimes, however, the dependence of the quasi-particle spectrum on the distribution function produces new effects which can rightly be called Fermi-liquid effects. We shall first consider the isotropic model of a metal in what follows for the sake of simplicity.

A new notation is used for the quasiparticle distribution function in this chapter, $n(\mathbf{p}, \mathbf{r})$. This is because the symbol f is conventionally used to denote the interaction function introduced by Landau in his theory of Fermi liquids.

Let us begin with the quasi-particle energy. Let $E[n]$ be the total energy of the system, $[n]$ denoting that the quantity considered is a functional of the distribution function. It is natural to define the energy of a quasi particle as follows. The change in total energy per

unit volume due to a change δn in the distribution function, is given by

$$\delta \left(\frac{E}{V} \right) = \sum_{\sigma} \int \varepsilon_{\sigma}(\mathbf{p}) \delta n_{\sigma}(\mathbf{p}) \frac{d^3 p}{(2\pi\hbar)^3}; \quad (1.22)$$

where we have included a summation over both spin orientations. The quantity $\varepsilon_{\sigma}(\mathbf{p})$ can be identified with the quasi-particle energy.

One should, in principle, include a position variable in addition to momentum and spin. In practice, however, variations of the distribution function over distances much larger than atomic dimensions, such as those discussed in previous chapters, will not affect quasi-particle energies, since the relevant electrons have wavelengths comparable to interatomic distances.

Equation (1.22) can be written in a slightly different form. If the spin of the electron plays an important role in the problem at hand, one must use the so-called density matrix $n(\mathbf{p}, \sigma)$ instead of the distribution function in (1.22). It can then be written in another form as

$$\delta \left(\frac{E}{V} \right) = \text{Tr}_{\sigma} \int \varepsilon(\mathbf{p}, \sigma) \delta n(\mathbf{p}, \sigma) \frac{d^3 p}{(2\pi\hbar)^3}, \quad (1.23)$$

where the trace (Tr) is taken with respect to the spin matrix. This definition of quasi-particle energy is consistent with a Fermi distribution function in equilibrium. The general expression $S = \sum [n \ln n + (1 - n) \ln (1 - n)]$ for the entropy is applicable to quasi-particles in a Fermi liquid is justified since it is based on purely combinatorial considerations involving Fermi statistics which hold for quasi particles just as for free particles in a Fermi gas. If we maximize the entropy subject to the requirements of constant energy and particle number, by varying the expression $S' = S + \alpha E + \beta N$ for entropy with respect to n , one finds

that $\delta S' = 0$ implies that $n(\varepsilon) = (e^{(\varepsilon-\mu)/T} + 1)^{-1}$, where μ and T can be related to α and β [3, 14].

1.6.2 The Landau Correlation Function (f)

A small change in the distribution function is accompanied by a small change in the quasi-particle energy itself, which can be written as [8]

$$\delta\varepsilon(\mathbf{p}, \hat{\sigma}, \mathbf{r}, t) = \text{Tr}_{\hat{\sigma}'} \int \left(\int VF(\mathbf{p}, \mathbf{r}, \hat{\sigma}; \mathbf{p}', \mathbf{r}', \hat{\sigma}') d^3\mathbf{r}' \right) \delta n(\mathbf{p}', \hat{\sigma}', \mathbf{r}, t) \frac{d^3\mathbf{p}'}{(2\pi\hbar)^3}.$$

Since the function F is the second variational derivative of the total energy per unit volume, as one can easily prove through Taylor expansion of the total energy $E[n]$ about the ground state distribution function, it must be symmetric with respect to the interchange $\mathbf{p}, \sigma \rightleftharpoons \mathbf{p}', \sigma'$. The function F is generally dependent on position vectors as well. According to Hartree-Fock approximation, the function F has a form

$$VF(\mathbf{p}, \mathbf{r}, \hat{\sigma}; \mathbf{p}', \mathbf{r}', \hat{\sigma}') = f(\mathbf{p}, \hat{\sigma}; \mathbf{p}', \hat{\sigma}') \delta_D(\mathbf{r} - \mathbf{r}') + \frac{e^2}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|},$$

so that, $\delta\varepsilon(\mathbf{p}, \hat{\sigma}, \mathbf{r}, t) = \text{Tr}_{\hat{\sigma}'} \int \left(f(\mathbf{p}, \hat{\sigma}; \mathbf{p}', \hat{\sigma}') + \int \frac{e^2}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}' \right) \delta n(\mathbf{p}', \hat{\sigma}', \mathbf{r}, t) \frac{d^3\mathbf{p}'}{(2\pi\hbar)^3}$, or

$$\delta\varepsilon(\mathbf{p}, \hat{\sigma}, \mathbf{r}, t) = \text{Tr}_{\hat{\sigma}'} \int f(\mathbf{p}, \hat{\sigma}; \mathbf{p}', \hat{\sigma}') \delta n(\mathbf{p}', \hat{\sigma}', \mathbf{r}, t) \frac{d^3\mathbf{p}'}{(2\pi\hbar)^3} + e\varphi(\mathbf{r}, t); \quad (1.24)$$

With $\delta_D(\mathbf{r} - \mathbf{r}')$ being the Dirac delta function. For spatially inhomogeneous distributions, the presence of the second addend in this equation which identifies the charged Fermi liquid from the neutral one, can be considered as the Coulomb self-consistent field potential energy $e\varphi(\mathbf{r}, t)$ with the self-consistent field potential $e\varphi(\mathbf{r}, t)$ given by

$$e\varphi(\mathbf{r}, t) = \text{Tr}_{\hat{\sigma}'} \int \int \frac{e}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} \delta n(\mathbf{p}', \hat{\sigma}', \mathbf{r}, t) \frac{d^3\mathbf{p}' d^3\mathbf{r}'}{(2\pi\hbar)^3}$$

and satisfies the usual Poisson equation.

The spin dependent Landau correlation function $f(p, \hat{\sigma}; p', \hat{\sigma}')$ can be written as

$$f(\mathbf{p}, \hat{\sigma}; \mathbf{p}', \hat{\sigma}') = \eta(\mathbf{p}, \mathbf{p}') + \hat{\sigma}_i \hat{\sigma}'_k \zeta_{ik}(\mathbf{p}, \mathbf{p}').$$

Since there is no preferred direction in the isotropic case and if the interaction of the spins has an exchange origin, the second term becomes $\hat{\sigma}_i \hat{\sigma}'_k \zeta_{ik}(\mathbf{p}, \mathbf{p}') = \hat{\sigma} \hat{\sigma}' \zeta(\mathbf{p}, \mathbf{p}')$.

Since, actually, the theory of Fermi liquid is valid only for values of momentum laying on the Fermi surface, we can represent the Landau correlation function ζ and η , as an expansion in complete set of orthonormalized functions $\vartheta(\mathbf{p})$ [9, 15]:

$$\eta = \sum_{n=0}^{\infty} \phi_n \vartheta(\mathbf{p}) \vartheta(\mathbf{p}').$$

In the case of spherical Fermi surface, the functions ζ and η appear to depend only on the angle θ between \mathbf{p} and \mathbf{p}' . So that, it is convenient to use the Legendre polynomial expansion. The factors ϕ_n represent parameters describing the phenomenological theory of the Fermi liquid, and are subjected to the definition from comparisons of results of theory with experiment.

The connection implied by (1.24) manifests itself in the kinetic equation. The quantity $\frac{d\mathbf{p}}{dt}$ is the force acting on a quasi-particle wave packet. In section 1.4 we assumed that it was due to the external field alone. But in the present case, the energy of a quasi particle acquires a dependence on position through its dependence on the distribution function n . This results, in an additional effective potential $\delta\varepsilon$, describing the self-consistent field set up by other quasi particles, which includes the Coulomb term $e\varphi$. So that, the gradient of this potential, being the force exerted on the quasi particle by the others, must be included

in $\frac{d\mathbf{p}}{dt}$. One must therefore take

$$\frac{d\mathbf{p}}{dt} = e\mathbf{E} + \frac{e}{c} \frac{\partial \varepsilon}{\partial \mathbf{p}} \times \mathbf{H} - \frac{\partial \delta \varepsilon}{\partial \mathbf{r}}. \quad (1.25)$$

The distribution function has the form

$$n(\varepsilon) = n_0(\varepsilon_0) + \frac{\partial n_0}{\partial \varepsilon} [\delta \varepsilon_1 - \psi + e\varphi].$$

Denoting $\delta \varepsilon_1(\mathbf{p}, \mathbf{r}, t)$ by Ψ , we obtain

$$n(\mathbf{p}, \mathbf{r}, t) = n_0(\varepsilon_0) + \frac{\partial n_0}{\partial \varepsilon} [\Psi(\mathbf{p}, \mathbf{r}, t) - \psi(\mathbf{p}, \mathbf{r}, t) + e\varphi(\mathbf{r}, t)]$$

for the distribution function, and for the quasiparticle energy ε we get

$$\varepsilon = \varepsilon_0(\mathbf{p}) + e\varphi(\mathbf{r}, t) + \Psi,$$

where $\Psi(\mathbf{p}, \mathbf{r}, t) = \text{Tr}_{\sigma'} \int f(\mathbf{p}, \hat{\sigma}; \mathbf{p}', \hat{\sigma}') \delta n(\mathbf{p}', \hat{\sigma}', \mathbf{r}, t) \frac{d^3 p'}{(2\pi\hbar)^3}$.

In our case, the Boltzmann kinetic equation (1.17) becomes

$$\frac{dn}{dt} = \frac{\partial n}{\partial t} + \mathbf{v} \frac{\partial n}{\partial \mathbf{r}} + \mathbf{F}_{ex} \frac{\partial n}{\partial \mathbf{p}} = -\frac{n_1}{\tau},$$

where $\mathbf{v} = \frac{d\mathbf{r}}{dt}$, $n_1 = n(\varepsilon) - n_0(\varepsilon) = -\frac{\partial n_0}{\partial \varepsilon} \psi$, and

$$\mathbf{F}_{ex} = \frac{d\mathbf{p}}{dt} = \frac{e}{c} \frac{\partial \varepsilon}{\partial \mathbf{p}} \times \mathbf{H} + e\mathbf{E} - \frac{\partial \delta \varepsilon}{\partial \mathbf{r}} \approx \frac{e}{c} \mathbf{v} \times \mathbf{H} + \frac{e}{c} \frac{\partial \Psi}{\partial \mathbf{p}} \times \mathbf{H} + e\mathbf{E} - \frac{\partial \Psi}{\partial \mathbf{r}}.$$

Using the fact that the self consistent electric field is too small as compared to the external

one, i.e., $-\frac{\partial \varphi}{\partial \mathbf{r}} = \mathbf{E}_1 \ll \mathbf{E}$, clearly, we obtain for the partial derivatives

$$\begin{aligned} \frac{\partial n}{\partial t} &\approx -\frac{\partial n_0}{\partial \varepsilon} \left[\frac{\partial \psi}{\partial t} - \frac{\partial \Psi}{\partial t} \right], \\ \frac{\partial n}{\partial \mathbf{r}} &= -\frac{\partial n_0}{\partial \varepsilon} \left[e\mathbf{E}_1 - \frac{\partial \Psi}{\partial \mathbf{r}} + \frac{\partial \psi}{\partial \mathbf{r}} \right], \end{aligned}$$

and

$$\frac{\partial n}{\partial \mathbf{p}} = \frac{\partial n_0}{\partial \varepsilon_0} \frac{\partial \varepsilon_0}{\partial \mathbf{p}} + \frac{\partial n_0}{\partial \varepsilon} \left[\frac{\partial \Psi}{\partial \mathbf{p}} - \frac{\partial \psi}{\partial \mathbf{p}} \right] \approx -\frac{\partial n_0}{\partial \varepsilon} \left[-\mathbf{v} - \frac{\partial \Psi}{\partial \mathbf{p}} + \frac{\partial \psi}{\partial \mathbf{p}} \right].$$

Finally, the linearized transport equation in presence of external magnetic and weak electric field, in the assumption that the self consistent electric field \mathbf{E}_1 is neglected due to the fact that it is very weak even compared to the weak external electric field \mathbf{E} is [5]

$$\frac{\partial \psi}{\partial t} + \frac{\partial \psi}{\partial \mathbf{r}} \cdot \mathbf{v} - e \mathbf{v} \cdot \mathbf{E} + \frac{\partial \psi}{\partial t_H} - \frac{\partial \Psi}{\partial t} = -\frac{\psi}{\tau}. \quad (1.26)$$

Here t_H as defined in last section. This equation is the Boltzmann kinetic equation which accounts for the fermi liquid effect.

Chapter 2

Semi classical quantization of energy levels in layered conductors

2.1 Behavior Of Electron in Magnetic Field

In this chapter we shall deal with phenomena in which the quantum-mechanical nature of electrons is really significant. We shall begin with the behavior of electrons in a static magnetic field. Let us consider a weak field at first. We note that throughout the discussion that follows we consider a single band, and drop explicit reference to the band index. This is done primarily to avoid confusion between the band index and the magnetic quantum number. Throughout this chapter $\varepsilon_n(p_z)$ is the n^{th} allowed energy of an electron in the given band, with momentum p_z

2.1.1 Pauli Paramagnetism

Each electron has a spin $\hbar s$ and an intrinsic magnetic moment $2\beta s$, where $\beta = e\hbar/2mc$ is the Bohr magneton. The projection of s on any fixed direction can only take on the values $\pm\frac{1}{2}$. An applied magnetic field polarizes the electronic magnetic moments, giving rise to a net magnetic moment. This effect is called spin or Pauli para-magnetism [3, 4, 16].

It is easy to find the corresponding susceptibility $\chi = \partial M/\partial H$. The potential energy of the magnetic moment of an electron in an applied magnetic field \mathbf{H} is $-2\beta sH$. If the spin of an electron is along the field direction, its energy is $\varepsilon - \beta H$, while it is $\varepsilon + \beta H$ if the spin

is opposite to the field. Since in the Fermi distribution, the energy appears together with the chemical potential as $\varepsilon - \mu$, we may assume instead that the energy is unaffected, but that the chemical potential becomes $\mu + \beta H$ for electrons with spins parallel to the field and $\mu - \beta H$ for those with spins antiparallel to the field. Through the determination of the number of electrons per unit volume for both spin orientations, given as usual by $N = \int f(\varepsilon) v(\varepsilon) d\varepsilon$, we can determine the total number of electrons per unit volume at temperature T with spin in the direction of the applied field N_+ and N_- in opposite direction:

$$N_{\pm} = \frac{1}{2} \int_{\mu \mp \beta H + kT}^{\mu + kT} f(\varepsilon) v(\varepsilon) d\varepsilon \quad (2.1)$$

and hence, for $T = 0$ total magnetic moment per unit volume will be given by

$$M = (N_+ - N_-)\beta \cong \beta^2 H \nu(\mu),$$

provided that $\beta H \ll \mu$. The magnetic susceptibility at (near) absolute zero is therefore

$$\chi = \beta^2 \nu(\mu). \quad (2.2)$$

This result appears to be correct at first sight even within the framework of Fermi liquid theory, however, according to the Landau theory of Fermi liquids, the energy spectrum itself can change if the distribution function changes, and this leads to nontrivial modifications in several situations. This expression can, therefore, be used for order of magnitude estimates only. Note that we took $T = 0$ for simplicity. The leading temperature corrections are of order $(kT/\mu)^2$ as usual and can, therefore, be safely neglected.

2.1.2 Level Quantization for a Free Electron in a Uniform Magnetic Field

A definite failure of the semiclassical model arises whenever the semiclassical theory predicts closed orbits for the electronic motion projected on a plane perpendicular to the field. When this happens, the energies of motion perpendicular to \mathbf{H} are quantized. To find these energy levels one must in principle return to the Schrodinger equation for an electron in the periodic crystalline potential in the presence of the magnetic field. The solution of this problem has been accomplished only in the simple case of free electrons (i.e., zero periodic potential) in a magnetic field. We describe the results in the free electron case below.

Let us consider the quantum mechanics of an electron in a uniform applied magnetic field. Replacing the momentum operator $\mathbf{p} = -i\hbar\nabla$ by its generalized counterpart $\mathbf{p} - (e/c)\mathbf{A}$, where \mathbf{A} is the vector potential, we can write the Hamiltonian as [13]

$$\mathcal{H} = \frac{1}{2m} \left(\hbar \frac{\nabla}{i} - \frac{e}{c} \mathbf{A} \right)^2.$$

The spin contribution $-2\beta s\mathbf{H}$ is omitted since it merely produces a constant shift of the levels by $\pm\beta H$. Taking \mathbf{H} to be along the z axis and if we work in a gauge such that $A_y = Hx$, $A_x = A_z = 0$, we get that in the solution of the Schrodinger equation $\mathcal{H}\psi = \varepsilon\psi$ the eigen value ε . i.e, the orbital energy levels of an electron (in a cubical box with sides of length L) is determined by two quantum numbers, n and p_z :

$$\varepsilon_n(p_z) = \frac{p_z^2}{2m} + \left(n + \frac{1}{2} \right) \hbar\omega_c = \frac{p_z^2}{2m} + \beta H (2n + 1), \quad (2.3)$$

where $\omega_c = eH/mc$ is the frequency of the classical motion. The quantum number n runs through all nonnegative integers, and p_z takes on the same values as in the absence of a magnetic field $p_z = \frac{2\pi\hbar n_z}{L}$ for any integral n_z .

Successive intervals of the original continuous spectrum (for a sample of large dimensions) in (p_x, p_y) at $H = 0$ now collapse into single level. Each one of these levels must therefore be highly degenerate, the degeneracy being proportional to H as shown below.

We have from (2.15) (to be discussed in section 2.2); for fixed extremal value of $p_z = p_{zm}$, $S_{n_m} = \frac{2\pi e\hbar H_{n_m}}{c} (n_m + \frac{1}{2})$. If we fix $H_{n_m} = H_{n_m+1} = H$, and raise the extremal quantum number from n_m to $n_m + 1$, the extremal area will also change accordingly by $\Delta S = S_{n_m+1} - S_{n_m} = \frac{2\pi e\hbar H}{c}$. This area corresponds to the area of a single Landau level. But for fixed p_z , the quantization of energy levels is independent of spin orientation, so that, there is one state (orbital) for both spin orientations (i.e, parallel and antiparallel to H), corresponding to an area $(\frac{2\pi\hbar}{L})^2$ of (p_x, p_y) space. Hence, if within an area ΔS , there are D orbitals, D being the degeneracy parameter, we can write $\frac{1}{(\frac{2\pi\hbar}{L})^2} = \frac{D}{\Delta S}$. Using the above result for ΔS , we obtain $D = \xi H$ [16], where $\xi = \frac{L^2 e}{2\pi\hbar c}$ is constant. So that the degeneracy parameter D , being the number of orbitals in each Landau level, is directly proportional to the strength of the static magnetic field H .

Therefore, the number of levels with energy (2.3) for a given n and p_z is $D = \frac{L^2 e H}{2\pi\hbar c}$. In field of a kilo-gauss, and a sample 1 cm on a side, this degeneracy will be about 10^{10} . The degeneracy reflects the fact that a classical electron with a given energy and p_z , spirals about a line parallel to the z - axis, which can have arbitrary x - and y - coordinates.

Since there is no component of Lorentz force along \mathbf{H} , the energy of motion in the z -direction is unaffected by the field. However, the energy of motion perpendicular to the field, which would be generally discrete spectrum $(p_x^2 + p_y^2)/2m$ (but continuous for a sample of large dimensions) if no field were present, is now quantized in steps of βH (or $\hbar\omega_c$). This phenomenon is called orbit quantization. The set of all levels with a given n (and arbitrary p_z) is referred to collectively as the n^{th} Landau level.

It must be added that the above results are only valid when the radius of classical circular motion of an electron with energy ε and momentum $\hbar k$ is not comparable with the cross-sectional dimensions of the box. For an electron with energy $\mu \gg \beta H$ and $p_z = 0$ the condition is

$$L \gg r_c = \frac{v_F}{\Omega_c} = \frac{cp_F}{eH}. \quad (2.4)$$

For a kilogauss field the results are applicable to samples with dimensions on the order of centimeters, but fail when the sample is still as large as 0.1 mm. Since the separation of Landau levels is proportional to H as shown above, the density of states in our case in which the field \mathbf{H} is along z -axis as a function of p_z and ε for each spin orientation, as can easily be checked [3], is

$$\nu(p_z) = \frac{2V}{(2\pi\hbar)^2} \frac{eH}{c} \quad \text{and} \quad \nu(\varepsilon) = \frac{2V}{(2\pi\hbar)^2} \frac{eH}{c} \frac{\partial p_z}{\partial \varepsilon} \quad (2.5)$$

respectively, where $V = L^3$ is the volume of the sample.

We shall not use the free electron results except to illustrate and test the validity of Onsager's theory of the magnetic levels in a periodic potential (i.e., in real metals). The theory of the de Haas-van Alphen effect, which generalizes the Landau free electron results

to Bloch electrons and bears directly on the problem of Fermi surface determination will be discussed in the next chapter.

2.1.3 Landau Diamagnetism

The motion of electrons in a metal is modified in the presence of a magnetic field. The electrons begin to move along helical trajectories, giving rise to an induced field opposite to the applied one. In other words, the change in the orbital motion of the electrons brought about by the applied magnetic field is responsible for diamagnetism [3].

This is actually a purely quantum-mechanical effect which disappears in the classical limit. According to classical mechanics the momentum of an electron in the presence of a magnetic field must be replaced by $\mathbf{p} - (e/c)\mathbf{A}$, where \mathbf{A} is the vector potential. The energy is then a function of that expression. Since thermodynamic quantities depend on the energy alone and are given by integrals over all momenta, one can take $\mathbf{p} - (e/c)\mathbf{A}$ as the new variable of integration. The resulting expressions will then be of the same form as in the absence of a magnetic field.

A finite diamagnetism does occur as a result of the discrete quantization of the energy levels of an electron in a magnetic field.

Let us calculate the thermodynamic potential [17] Ω , ($d\Omega = -\mathcal{P}dV - SdT - Nd\mu - MdH$), involving Fermi-Dirac distribution function through $N = \sum_i n_o(\varepsilon_i) = \sum_i \left(e^{\frac{\varepsilon_i - \mu}{kT}} + 1 \right)^{-1}$. The general expression of Ω for a system electrons is

$$\Omega = -kT \sum_i \ln [1 + e^{(\mu - \varepsilon_i)/kT}], \quad (2.6)$$

where the summation is over all quantum states (n_z or p_z and n in our case). After passing from summation over p_z to integration by using our density of states (2.5), it becomes

$$\Omega = -\frac{4kTeHV}{(2\pi\hbar)^2 c} \sum_n \int \frac{\partial \epsilon}{\partial p_z} dp_z \ln [1 + e^{(\mu-\epsilon)/kT}].$$

Integrating by parts, and substituting $p_z(\epsilon, n) = \pm \{2m[\epsilon - \beta H(2n+1)]\}^{1/2}$, which follows from (2.3), one finds

$$\Omega = -\frac{4VeH}{(2\pi\hbar)^2 c} \sum_n \int_{\beta H(2n+1)}^{\mu} (2m)^{1/2} d\epsilon [\epsilon - \beta H(2n+1)]^{1/2}, \quad (2.7)$$

where the sum over n is restricted by the condition $\epsilon > \beta H(2n+1)$ and the factor 2 takes into account the freedom of taking either sign in $p_z(\epsilon, n)$.

Expression (2.7) is valid at all temperatures. The integral can easily be evaluated at temperatures such that $kT \ll \mu$ as one may set $T = 0$, since corrections will be of order $(kT/\mu)^2$ in the weak field limit. We, therefore, approximate the Fermi distribution by a step-function and interchange the order of the summation over n and integration over ϵ , so that

$$\Omega = -\frac{8}{3} \frac{VeH}{(2\pi\hbar)^2 c} (2m)^{1/2} \sum_{n < \frac{\mu}{2\beta H} - \frac{1}{2}} [\mu - \beta H(2n+1)]^{3/2}.$$

For small H (weak field limit) this sum can be replaced by an integral by means of the Euler-MacLaurine formula [7],

$$\sum_{n=0}^{n_o} f(n) = \int_{-1/2}^{n_o+1/2} f(n) dn - [f'(n_o+1/2) - f'(-1/2)]/24, \quad (2.8)$$

so that one gets for Ω , after substituting $\beta = e\hbar/2mc$ and $\mu = p_o/2m$,

$$\Omega = -\frac{p_o^5 V}{15m\pi^2 \hbar^3} + \frac{V\beta^2 H^2}{6} \frac{p_o m}{\pi^2 \hbar^3}. \quad (2.9)$$

The magnetic moment per unit volume is thus

$$M = -\frac{1}{V} \frac{\partial \Omega}{\partial H} = -\beta^2 \frac{H}{3} \frac{p_o m}{\pi^2 \hbar^3}, \quad (2.10)$$

and the magnetic susceptibility is, therefore, $\chi = -\frac{\beta^2}{3} \frac{p_o m}{\pi^2 \hbar^3}$. But we know that the quantity $p_o m / \pi^2 \hbar^3$ is just the free-electron density of states $\nu(\mu)$, so that the diamagnetic contribution to the susceptibility is

$$\chi_{\text{dia}} = -\frac{\beta^2}{3} \nu(\mu). \quad (2.11)$$

Comparing this with $\chi_{\text{para}} = \beta^2 \nu(\mu)$ determined in the last section, we conclude that the diamagnetic susceptibility due to the quantization of electronic levels in a magnetic field is 1/3 of the paramagnetic spin susceptibility for a free-electron gas. Such a gas must therefore exhibit a net para-magnetism.

Many diamagnetic metals do occur in nature, however. Consider, for instance, the simplest case of an isotropic spectrum $\varepsilon = p^2/2m^*$ with an isotropic effective mass m^* . The quantities β appearing in χ_{dia} is related to the orbital motion of the electrons, so that it must be replaced by $\beta^* = e\hbar/2m^*c$ and $\chi_{\text{dia}} = -\frac{\beta^{*2}}{3} \nu(\mu)$, but β stands for the actual Bohr magneton in $\chi_{\text{para}} = \beta^2 \nu(\mu)$, which involves the free-electron mass. Thus, we have

$$|\chi_{\text{dia}}/\chi_{\text{para}}| = \frac{1}{3} (m/m^*)^2, \quad (2.12)$$

which may well exceed 1 in some cases.

2.2 Semiclassical Quantization of Energy Levels For an Arbitrary Electronic System

We shall not discuss expression (2.7) in the high field limit at finite temperature, since, as noted there, the most interesting consequences can be obtained for an arbitrary electronic spectrum and do not apply to the free electronic model alone. The exact energy levels cannot, of course, be determined in the general case. Onsager's generalization of Landau's free electron result is only valid for magnetic levels with fairly high quantum numbers [3]. Thus, we shall find that the de Haas-van Alphen effect is due to levels at Fermi energy which almost always do have very high quantum numbers. Comparing the separation βH between Landau levels with the chemical potential μ one finds $\beta H/\mu \simeq \hbar\omega/\mu = \hbar^2 e \hbar H / m c \mu \sim 10^{-4}$ for typical laboratory fields ($\sim 10^4$ G). Unless almost all the electronic energy is in motion parallel to the field, a level of energy μ must have a corresponding quantum number n whose order of magnitude is $\mu/\beta H$ which will be of order 10^4 in the said field.

Generally, for arbitrary energy spectrum $\mu \gg \beta H$, from which it follows that, the relevant states must have high quantum numbers; we can apply the semi classical Bohr quantization rule [18]. Energies of levels with very high quantum numbers can be accurately calculated with Bohr's correspondence principle, which asserts that the difference in energy of two adjacent levels is Planck's constant times the frequency of classical motion at the energy of the levels. Since p_z is a constant of the semiclassical motion, we apply this condition to levels with a specified p_z , and quantum numbers n and $n + 1$.

Under the application of a static magnetic field $\mathbf{H} = (0, 0, H)$, the quasi momentum \mathbf{p} of an electron (here considered as quasi particle), has to be replaced by the canonical momentum \mathbf{P} conjugate to the canonical coordinate \mathbf{r} as

$$\mathbf{P} = \mathbf{p} - \frac{e}{c} \mathbf{A}. \quad (2.13)$$

Without loss of generality of results, the vector potential \mathbf{A} can be chosen in the Landau gauge [19], in which $\mathbf{A} = (0, Hx, 0)$, so that, we can write $P_x = -\frac{\hbar}{i} \frac{\partial}{\partial x}$, and $P_y = \frac{\hbar}{i} \frac{\partial}{\partial y} - \frac{eH}{c} x$ and it follows that $[P_x, P_y] = P_x P_y - P_y P_x = i\hbar \frac{eH}{c}$. Now, suppose that Y plays the role of the generalized coordinate conjugate to P_y , i.e., $[Y, P_y] = i\hbar$. Comparing this with the last equation, we obtain $Y = \frac{c}{eH} P_x$. For closed orbit the Bohr quantization rule gives

$$\oint P_y dY = \oint P_y d\left(\frac{c}{eH} P_x\right) = 2\pi\hbar (n + \gamma(n)), \quad (2.14)$$

$\gamma(n)$ being a slowly varying function of n ($0 < \gamma(n) < 1$). Using the definition of Y , one finds

$$\oint P_y dP_x = \frac{2\pi\hbar eH}{c} (n + \gamma(n)).$$

From Green's theorem we have $\oint_C P_y dP_x = - \iint_S dP_x dP_y = \iint_S dS_n = S_n$. This expression is simply the area enclosed by the orbit in momentum space and should be normal to the field direction. Electrons traverse the orbit C , leaving the surface S_n enclosed by the orbit, to the right. Such an orbit is defined by the conditions $p_z = \text{constant}$, $\varepsilon = \text{constant}$, i.e., is the intersection of a constant energy surface with the plane $p_z = \text{constant}$ (see section 1.5). We have, therefore,

$$S(\varepsilon, p_z) = \frac{2\pi\hbar eH}{c} (n + \gamma(n)). \quad (2.15)$$

2.2 Semiclassical Quantization of Energy Levels For an Arbitrary Electronic System 42

For free electrons $S(\varepsilon, p_z) = \pi(p^2 - p_z^2) = \pi(2m\varepsilon - p_z^2)$, which gives $\varepsilon = p_z^2/2m + \frac{2\pi\hbar eH}{2mc} (n + \gamma(n))$ in agreement with (2.3)

It is easy to find the area enclosed by the orbit A_n in the real space (using the ideas in section 1.5) $S_n(\varepsilon, p_z) = -\left(\frac{e}{c}H\right)^2 \oint_C xdy = \left(\frac{e}{c}H\right)^2 \left(-\int_S dx dy\right) = \left(\frac{e}{c}H\right)^2 A_n$.

Energies of levels with very high quantum numbers can be accurately calculated so as to rederive (2.15) with Bohr's correspondence principle, which asserts that the difference in energy of two adjacent levels is Planck's constant times the frequency of classical motion at the energy of the levels. Since p_z is a constant of the semiclassical motion, we apply this condition to levels with a specified p_z , and quantum numbers n and $n + 1$.

Let $\varepsilon_n(p_z)$ be the energy of the n^{th} allowed level at the given p_z . The correspondence principle then gives

$$\varepsilon_{n+1}(p_z) - \varepsilon_n(p_z) = \frac{2\pi\hbar}{T(E_n(p_z), k_z)},$$

where $T(E, p_z)$ is the period of semiclassical motion on the orbit specified by ε , and p_z (see (1.21)) determined in the semiclassical model) $T(\varepsilon, p_z) = \frac{2\pi c}{eH} \frac{\partial S(\varepsilon, p_z)}{\partial \varepsilon}$. Combining the last two equations, we may write

$$(\varepsilon_{n+1}(p_z) - \varepsilon_n(p_z)) \frac{\partial S(\varepsilon)}{\partial \varepsilon} = \frac{2\pi e\hbar H}{c}.$$

Because we are interested in ε of the order of μ , we can greatly simplify this equation. On the basis of the free electron results we expect that the energy difference between neighboring Landau levels will be of order $\hbar\omega_c$ which is much smaller than the energies of the levels themselves, as discussed earlier. It is therefore an excellent approximation to

take $\frac{\partial S(\varepsilon_n, p_z)}{\partial \varepsilon} = \frac{S(\varepsilon_{n+1}, p_z) - S(\varepsilon_n, p_z)}{\varepsilon_{n+1} - \varepsilon_n}$ and substituting this in the previous expression we find

$$S(\varepsilon_{n+1}, p_z) - S(\varepsilon_n, p_z) \equiv \Delta S = 2\pi e\hbar H/c. \quad (2.16)$$

which is equivalent to (2.15) and states that classical orbits at adjacent allowed energies (and the same p_z) enclose areas that differ by the fixed amount $\Delta S(\varepsilon_n, p_z) = \frac{2\pi e\hbar H}{c}$.

According to the discussion in Chap.1 Sec.5, the projection of the trajectory of an electron in real space on the (x, y) plane has the same shape as the orbit in momentum space, the corresponding area being $(c/eH)^2 S$. According to (2.16) the change in this area in going from the n^{th} to the $(n+1)^{\text{st}}$ level is $\Delta A = (c/eH)^2 \Delta S = \frac{2\pi c\hbar}{eH}$. Multiplying by H we find the corresponding change in magnetic flux corresponding change in the magnetic flux is $\Delta\Phi_H = H\Delta A$,

$$\Delta\Phi_H = 2\pi c\hbar/e = \Phi_0. \quad (2.17)$$

This result is independent of any variable and is expressed in terms of universal constants and is known as the magnetic flux quantum Φ_0 : $\Phi_0 = \frac{2\pi\hbar c}{e} = 4 \times 10^{-7} \text{ G cm}^2$. This shows that the allowed Landau levels must be such that the difference between the magnetic flux through the associated orbits is equal to an integral number of flux quanta.

Another way of stating this conclusion is that; for large value of n , the area enclosed by the semiclassical orbit at an allowed energy and p_z , must depend on n according to

$$S(\varepsilon_n(p_z), p_z) = (n + \lambda) \Delta S, \quad (2.18)$$

where λ is independent of n . This is Onsager's famous result [18], which he derived by an alternate method, using the Bohr-Sommerfeld quantization condition.

Chapter 3

The De Haas-Van Alphen Effect

In 1930 de Haas and van Alphen [1] measured the magnetization M of a sample of bismuth as a function of magnetic field in high fields at 14.2 K, and found oscillations in M/H .

This phenomenon, observed only at low temperatures and high fields is an important key to the electron structure of metals. The full extent of its usefulness was only pointed out in 1952, by Onsager. Since the original experiment, and especially since around 1960, careful observations have been made in many metals of this same oscillatory field dependence on the magnetic susceptibility, $\chi = dM/dH$.

The oscillations display a remarkable regularity if the susceptibility is plotted not against field but against inverse field. It then becomes clear that χ has a periodic dependence on $1/H$, though frequently two or more periods are superposed. Similar oscillatory behavior has been observed not only in the susceptibility, but also in the conductivity (Shubnikov-de Haas effect) [20] and others.

Two major techniques have been widely exploited to measure the oscillations. One, based on the fact that in a field, a magnetized sample experiences a torque proportional to its magnetic moment. This torque simply measures the oscillations, in angular position of the sample attached to a filar suspension, as the magnetic field strength, and hence the magnetization $M(H)$ varies. The second technique, especially valuable if high fields are

required, measures the voltage induced in a pickup coil surrounding the sample when a burst of field is applied.

Even before the key to the theory of the de Haas-van Alphen effect for Bloch electrons was pointed out by Onsager, Landau 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 (see 2.1.2) [21]. The phenomenon became of even greater interest and importance when Onsager pointed out that the change in $1/H$ through a single period of oscillation $\Delta(1/H)$ was determined by the remarkably simple relation.

In this chapter we will summarize the general theoretical result developed by Onsager, Landau and Abrikosov, and then apply this theory to special case of definite type of energy spectrum. In particular we analyze the results for a quasi two dimensional energy spectrum of quasiparticles (layered conductor). As an example, we take corrugated cylinder type Fermi surface (1.8) for quantitative comparison with spherical one. The account of the Fermi liquid effect will also be considered in evaluation of the magnetic susceptibility.

In chapter 2 we found the magnetic susceptibility of the free-electron gas. In the approximation considered there we relied on the lowest correction of order $(\beta H/\mu)^2$ to the thermodynamic potential due to the magnetic field. We shall now derive the next higher order correction. We shall see that it is a rapidly oscillating function of the magnetic field, so that its derivative with respect to H can exceed the non oscillatory part of the magnetic moment at sufficiently low temperatures.

We shall present a calculation valid for an arbitrary electronic energy spectrum. Appropriate formulas for the energy levels and the corresponding density of states were obtained in the preceding chapter

3.1 The Thermodynamic Potential

Before going to the important details, we first have to determine the thermodynamic potential which naturally arises in the statistical mechanics theory of a single component simple system known as the grand canonical potential $\Omega = U[T, \mu]$, involving Fermi-Dirac distribution function through $N = \sum_i n_o(\varepsilon_i) = \sum_i \left(e^{\frac{\varepsilon_i - \mu}{kT}} + 1 \right)^{-1}$. The thermodynamic potential itself is given by (2.7) which in our case becomes:

$$\Omega = -\frac{VeHkT}{c(2\pi\hbar)^2} \sum_{n, \sigma_z} \int \ln \left(e^{\frac{\mu_{\sigma_z} - \varepsilon_n(p_z)}{kT}} + 1 \right) dp_z. \quad (3.1)$$

The index σ_z runs over the two allowed spin orientations, and $\mu_{\sigma} = \mu \pm \sigma_z \beta H$. To evaluate the integral in (3.1) we can use Poisson sum formula [7]

$$\sum_{n=0}^{\infty} f(n) = \int_{-\gamma}^{\infty} f(n) dn + 2 \operatorname{Re} \sum_{l=1}^{\infty} \int_{-\gamma}^{\infty} f(n) e^{2\pi i n l} dn \quad (3.2)$$

which holds in our case for γ between -1 and 0 . Applying Poisson's formula (3.2) to the sum in (3.1) we obtain two integrals: the first is the non oscillatory Ω^{nosl} and the second corresponds to the oscillatory contribution Ω^{osl} . Letting $\gamma = 0$, our Ω will be the sum of the two terms:

$$\Omega = \Omega^{\text{nosl}} + \Omega^{\text{osl}} = - \sum_{\sigma_z} I_{\sigma_z} - 2 \operatorname{Re} \sum_{\sigma_z l} I_{\sigma_z l},$$

where

$$I_{\sigma_z} = \frac{VeHkT}{c(2\pi\hbar)^2} \int_0^\infty dn \int dp_z \ln \left(e^{\frac{\mu_{\sigma_z} - \epsilon_n(p_z)}{kT}} + 1 \right)$$

and

$$I_{\sigma_z l} = \frac{VeHkT}{c(2\pi\hbar)^2} \int_0^\infty dn \int dp_z e^{2\pi i n l} \ln \left(e^{\frac{\mu_{\sigma_z} - \epsilon_n(p_z)}{kT}} + 1 \right) dp_z. \quad (3.3)$$

We are interested in the oscillating part, Ω^{osl} , since it is involved in the oscillation of magnetization and hence in the de-Haas-Van-Alphen effect. Therefore, we pay much of our attention on that term:

$$\Omega^{\text{osl}} = -2 \text{Re} \sum_{\sigma_z s} I_{\sigma_z l}. \quad (3.4)$$

Changing now the integration over n to an integration over energy, we have for the p_z integral $\int dn \int e^{2\pi i n l} f(\epsilon, p_z) dp_z = \int d\epsilon \int f(\epsilon, p_z) dp_z \frac{\partial n}{\partial \epsilon} e^{2\pi i n l}$. The factor $e^{2\pi i n l}$ in this p_z integral is a rapidly oscillating function. If $n(\epsilon, p_z)$ achieves an extremal value $n_q(\epsilon)$ for a particular value p_z , say p_{zq} , by expanding $n(\epsilon, p_z)$ in Taylor series, in powers of $p_z - p_{zq}$ and neglecting terms above the second order and noting that $\left(\frac{\partial n}{\partial p_z}\right)_q = 0$, one gets $n(\epsilon, p_z) \approx n_q(\epsilon) + \frac{1}{2} \left(\frac{\partial^2 n}{\partial p_z^2}\right)_q (p_z - p_{zq})^2$. Noting that only these extrema make significant contributions to the p_z integration, in the vicinity of a particular extremum, this integral can be approximated as follows:

$$I = \left(\frac{\partial^2 n}{\partial p_z^2}\right)_q e^{2\pi i n l} \int dx \exp \left\{ i l \left(\frac{\partial^2 n}{\partial p_z^2}\right)_q x^2 \right\},$$

where $x = p_z - p_{zq}$. The value of this integral depends on the sign of $\left(\frac{\partial^2 n}{\partial p_z^2}\right)_q$.

Taking $y = \exp\left(i\pi \operatorname{signum}\left[\left(\frac{\partial^2 n}{\partial p_z^2}\right)_q\right]\right) x$ we obtain $I = e^{\pm\pi/4} \left\{ \left(l \left(\left| \frac{\partial^2 n}{\partial p_z^2} \right| \right)_q \right)^{-1/2} \right\}$,

so that

$$I_{\sigma_z l} \cong \frac{VeHkT}{c(2\pi\hbar)^2} \sum_q e^{\pm i\pi/4} \int d\varepsilon \ln \left(e^{\frac{\mu_{\sigma_z} - s_n(p_z)}{kT}} + 1 \right) e^{2\pi i n_q l} \frac{\partial n_q}{\partial \varepsilon} \left(l \left(\left| \frac{\partial^2 n}{\partial p_z^2} \right| \right)_q \right)^{-1/2}, \quad (3.5)$$

where the sum includes all extremal values n_q . Integrating by parts, and taking into account that only the logarithm and $e^{2\pi i n_q l}$ are rapidly varying functions of ε , so that all remaining factors can be treated as constant, one obtains

$$I_{\sigma_z l} \cong \frac{VeHkT}{c(2\pi\hbar)^2} \frac{1}{2\pi l^{3/2}} \sum_q e^{\pm i\pi/4} \int \frac{e^{2\pi i n_q l}}{e^{\frac{s_n(p_z) - \mu_{\sigma_z}}{kT}} + 1} d\varepsilon \frac{\partial n_q}{\partial \varepsilon} \left| \frac{\partial^2 n}{\partial p_z^2} \right|_q^{-1/2} \quad (3.6)$$

for the oscillatory contribution.

The main contribution to the integral comes from the vicinity of $\varepsilon = \mu$. Although $e^{2\pi i n_q l}$ is rapidly oscillating, n_q itself is a smooth function which can be expanded about μ_{σ_z} , i.e., $n_q(\varepsilon) \cong n_q(\mu_{\sigma_z}) + (\partial n_q / \partial \varepsilon)_{\mu_{\sigma_z}} (\varepsilon - \mu_{\sigma_z})$, so that

$$\int \frac{e^{2\pi i n_q l}}{e^{\frac{\varepsilon - \mu_{\sigma_z}}{kT}} + 1} d\varepsilon \cong e^{2\pi i n_q(\mu_{\sigma_z}) l} \int_{-\infty}^{\infty} \frac{e^{2\pi i l x (\partial n_q / \partial \varepsilon)_{\mu_{\sigma_z}}}}{e^{\frac{x}{kT}} + 1} dx,$$

in which the limit of ε integration from $\mu - \beta H$ to $\mu + \beta H$ when passing to the $x = \varepsilon - \mu_{\sigma_z}$ becomes from $-\infty$ to ∞ for large H . Thus, using $\int_{-\infty}^{\infty} \frac{e^{iay}}{e^y + 1} dy = -\frac{i\pi}{\sinh(\pi a)}$, one gets

$$I_{\sigma_z l} \cong \frac{-2VeHkT}{2\pi c(2\pi\hbar)^2 l^{3/2}} \sum_q e^{\pm i\pi/4} \left| \frac{\partial^2 n}{\partial p_z^2} \right|_{q, \mu_{\sigma_z}}^{-1/2} \frac{e^{2\pi i n_q(\mu_{\sigma_z}) l}}{\sinh\left(2\pi^2 l (\partial n_q / \partial \varepsilon)_{\mu_{\sigma_z}}\right)}. \quad (3.7)$$

When this expression is inserted into (3.4), one must perform the spin summation. Since the only rapidly oscillating factor is $e^{2\pi i n_q(\mu_{\sigma_z}) l}$. From $\mu_{\sigma_z} = \mu \pm \beta H$, recalling that $\mu \gg \beta H$, we can set $\mu_{\sigma_z} = \mu$ in all the remaining terms. Expanding $n_q(\mu_{\sigma_z})$ about μ in

the exponent under sum, one obtains

$$\begin{aligned} \sum_{\sigma_z} \exp(2\pi i n_q(\mu_{\sigma_z}) l) &\cong e^{2\pi i n_q(\mu) l} \sum_{\sigma_z} \exp\left(2\pi i l (\partial n / \partial \varepsilon)_\mu \sigma_z \beta H\right) \\ &= 2e^{2\pi i n_q(\mu) l} \cos\left(2\pi l (\partial n / \partial \varepsilon)_\mu \beta H\right). \end{aligned}$$

According to (2.15) $n_q(\mu) \cong \frac{c}{2\pi e \hbar H} S_q$, $\frac{\partial^2 n}{\partial p_z^2} = \frac{c}{2\pi e \hbar H} \frac{\partial^2 S}{\partial p_z^2}$ and $(\partial n_q / \partial \varepsilon)_\mu = \frac{c}{2\pi e \hbar H} \left(\frac{\partial S}{\partial \varepsilon}\right)_{q,\mu} = m_q^*(\mu, p_{zq}) \frac{c}{e \hbar H}$. Hence, the oscillatory part of the thermodynamic potential becomes (with $\beta = e \hbar / 2mc$),

$$\begin{aligned} \Omega^{\text{osl}} &\cong \frac{V \left(\frac{e \hbar H}{c}\right)^{5/2}}{2^{3/2} \pi^{7/2} \hbar^3} \times \\ &\sum_{q,l} \left| \frac{\partial^2 S}{\partial p_z^2} \right|_{q,\mu}^{-\frac{1}{2}} \frac{\Lambda(l \lambda_q)}{[m_q^*(\mu, p_{zq})] l^{5/2}} \cos\left(\pi l \frac{m_q^*(\mu, p_{zq})}{m}\right) \cos\left(l \frac{c S_q}{e \hbar H} \pm \pi/4\right) \end{aligned} \quad (3.8)$$

where $m_q^* = \frac{1}{2\pi} (\partial S / \partial \varepsilon)_{\mu, p_{zq}}$, $\lambda_q = \frac{2\pi^2 k T c m_q^*(\mu, p_{zq})}{e \hbar H}$ and $\Lambda(Z) = \frac{Z}{\sinh Z}$ and the sum over q extends over all the extremal cross-sectional areas of the Fermi surface whereas the sum over l is from 1 to ∞ .

3.2 The Oscillation of Magnetization

Let us estimate the relative importance of oscillatory contributions to various thermodynamic quantities. Consider the ratio of Ω^{osl} and Ω_0 , the thermodynamic potential for $H = 0$.

We can estimate Ω_0 as follows [3]

$$\Omega_0 \sim V n \mu \sim V \left(\frac{p_0}{\hbar}\right)^3 \frac{p_0^2}{m} \mu \sim V S^{5/2} \frac{p_0^2}{m \hbar^3}.$$

Now $\Omega^{\text{osl}} / \Omega_0 \sim \left(\frac{2\pi e \hbar H}{c S}\right)^{5/2} \sim \left(\frac{\beta H}{\mu}\right)^{5/2}$ is a small quantity. The non oscillatory contribution to Ω due to the magnetic field is of the order $\left(\frac{\beta H}{\mu}\right)^2$. The oscillatory part is therefore small even compared to that contribution.

Consider now the importance of the oscillatory contribution to the magnetization,

$$M^{\text{osl}} = -\frac{1}{V} \frac{\partial \Omega^{\text{osl}}}{\partial H}. \quad (3.9)$$

According to (3.8) one obtains

$$M^{\text{osl}} \approx \frac{-(\frac{e\hbar}{c})^{3/2} H^{1/2}}{2^{3/2} \pi^{7/2} \hbar^3} \sum_q \left| \frac{\partial^2 S_q}{\partial p_z^2} \right|_q^{-1/2} \frac{S_q}{m_q^*} \sum_l \frac{\Lambda(l\lambda_q)}{l^{3/2}} \sin\left(l \frac{cS_q}{e\hbar H} \pm \pi/4\right) \cos\left(\pi l \frac{m_q^*}{m}\right). \quad (3.10)$$

At low temperatures $\Lambda(l\lambda_q) \sim 1$ ($\lim_{x \rightarrow 0} \frac{x}{\sinh(x)} = 1$), and $M^{\text{osl}} \sim \frac{H^{1/2}}{\hbar^3} \left(\frac{e\hbar}{c}\right)^{3/2} \frac{S}{m}$. The non oscillatory contribution to the magnetization is $M_0 \sim \left(\frac{\beta^2}{\hbar^3}\right) p_0 m H$ and thus $M^{\text{osl}}/M_0 \sim \left(\frac{\beta}{\mu}\right)^{1/2}$. This shows that the oscillatory contribution is more important than the non oscillatory one at low temperatures. This is due to the high frequency of the oscillations which enhances the effect upon differentiation.

If the temperature is not too low, only the first term in the sum over l is significant so that taking $l = 1$, $\frac{\Lambda(l\lambda_q)}{l^{3/2}} = \Lambda(\lambda_q) \approx \frac{\lambda_q}{\sinh \lambda_q} = \frac{2e^{\lambda_q} \lambda_q}{e^{2\lambda_q} - 1} \approx 2\lambda_q e^{-\lambda_q} = 2 \frac{2\pi^2 kT c m_q^*}{e\hbar H} e^{-\frac{2\pi^2 kT c m_q^*}{e\hbar H}}$ we have

$$M^{\text{osl}} \approx \frac{-2^{1/2} \left(\frac{e\hbar}{c}\right)^{1/2} kT}{\pi^{3/2} \hbar^3 H^{1/2}} \sum_q S_q \left| \frac{\partial^2 S_q}{\partial p_z^2} \right|_q^{-1/2} e^{-\frac{2\pi^2 kT c m_q^*}{e\hbar H}} \sin\left(\frac{cS_q}{e\hbar H} \pm \frac{\pi}{4}\right) \cos\left(\pi \frac{m_q^*}{m}\right) \quad (3.11)$$

The magnetization oscillations are periodic in H^{-1} , the period being

$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e\hbar}{cS_q} \quad (3.12)$$

This equation could also be derived using (2.15) $S(\varepsilon, p_z) = \frac{2\pi\hbar eH}{c} (n + \gamma(n))$ putting $\gamma = 1/2$. The extremal crosssectional area on the Fermi surface corresponding to the n_q^{th} quantum number where the corresponding magnetic field is H_{n_q} can be written as $S_{n_q} =$

$\frac{2\pi\hbar e H_{nq}}{c} \left(n_q + \frac{1}{2}\right)$, or $\frac{1}{H_{nq}} = \frac{2\pi\hbar e}{cS_{nq}} \left[n_q + \frac{1}{2}\right]$. Fixing the extremal area at S_{nq} , if we vary the magnetic field to $H_{(n_q+1)}$, we get $\frac{1}{H_{(n_q+1)}} = \frac{1}{H_{nq}} + \frac{2\pi\hbar e}{cS_{nq}}$. Therefore, the magnetization oscillation is periodic in $\frac{1}{H}$ with a period $\Delta\left(\frac{1}{H}\right) = \frac{1}{H_{(n_q+1)}} - \frac{1}{H_{nq}} = \frac{2\pi\hbar e}{cS_{nq}}$.

At low temperatures the other terms in the sum over l in (3.10) cannot be neglected. The period of the magnetization oscillations is nevertheless still given by (3.12).

We obtained the final formula for the De Haas-Van Alphen oscillations after a rather long-winded derivation. The physical reason for their origin is easily explained if one considers how successive electronic levels are filled.

3.3 Application to Layered Conductors

Consider now the less general case when the energy spectrum is quasi two dimensional, of the form discussed in section 1.1. The results obtained above hold true only for external static field, but consideration of the Bloch electron generally does not affect these results qualitatively. Under the application of a static magnetic field $\mathbf{H} = (0, 0, H)$, the quasi momentum \mathbf{p} of an electron has to be replaced by the canonical momentum \mathbf{P} conjugate to the canonical coordinate \mathbf{r} . However, if the condition of quantization is fulfilled, and if the field direction is in the direction of the openness of our cylinder, there will not be a change in the form of the energy as compared to the free electron result (2.3). The only expected difference is that, the degeneracy dependence on the form of the Fermi surface $\varepsilon = \mu$, which exhibits through the density of states. It is clear that this also affects the magnetic susceptibility.

Consider the simplest quadratic energy spectrum (1.8)

$$\varepsilon(\mathbf{p}) = \frac{p_x^2 + p_y^2}{2m} + \varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right), \quad (3.13)$$

i.e., we have $\varepsilon_1 \cos(\frac{ap_z}{\hbar})$ instead of $\frac{p_z^2}{2m}$ in (2.3), since the magnetic field is along p_z . The orbit of electrons for a given p_z will be circular and the cross-section S is circular ($S = 2m\pi (\varepsilon - \varepsilon_1 \cos(\frac{ap_z}{\hbar}))$). There will be two extrema within a Brillouin zone, one maxima and one minima. Exremal areas correspond to the two exremal diameters of our cylinder at $p_{zq} = \frac{\pi\hbar}{a}q$, for any two consecutive values of q . So that, in all equations, S_q will be $2\pi m (\mu - (-1)^q \varepsilon_1)$. The cyclotron mass $m_q^* = \frac{1}{2\pi} (\partial S / \partial \varepsilon)_{\mu, p_{zq}}$ is the same as the mass m , where as $\left| \frac{\partial^2 S}{\partial p_z^2} \right|_{q, \mu}^{-\frac{1}{2}} = \frac{\hbar}{a(2m\pi\varepsilon_1)^{\frac{1}{2}}}$. In (3.11), for maxima both $(-1)^q$ and (\pm) attain $(-)$; and for minima, they attain $(+)$; along with this, one has to take

$$S_q = 2\pi m (\mu - (-1)^q \varepsilon_1), \quad m_q^* = m, \quad \left| \frac{\partial^2 S}{\partial p_z^2} \right|_{q, \mu}^{-\frac{1}{2}} = \frac{\hbar}{a(2m\pi\varepsilon_1)^{\frac{1}{2}}}, \quad (3.14)$$

for both exremals. Substituting these in (3.11) we have for the oscillatory part of the magnetization,

$$M^{\text{osl}} \cong \frac{2 \left(\frac{e\hbar}{c}\right)^{1/2} m^{\frac{1}{2}} kT}{\pi \hbar^2 a H^{1/2} \varepsilon_1^{\frac{1}{2}}} \exp\left(-\frac{\pi^2 kT}{\beta H}\right) \sum_{-,+} (\mu \pm \varepsilon_1) \sin\left(\frac{\pi(\mu \pm \varepsilon_1)}{\beta H} \mp \frac{\pi}{4}\right), \quad (3.15)$$

where the sum is over the two extrema (i.e., $(\mu \pm \varepsilon_1)$ and $\mp \frac{\pi}{4}$ attain $(\mu + \varepsilon_1)$ and $(-\frac{\pi}{4})$, or $(\mu - \varepsilon_1)$ and $(+\frac{\pi}{4})$ respectively at a time) and we see that there are two periods of oscillation:

$$\Delta \left(\frac{1}{H}\right)_{\text{min}} = \frac{2\beta}{(\mu + \varepsilon_1)}, \quad \Delta \left(\frac{1}{H}\right)_{\text{max}} = \frac{2\beta}{(\mu - \varepsilon_1)}, \quad (3.16)$$

for minima and maxima respectively which superimpose. In figure (3.2) based on (3.15) a theoretical plot of M/H verses H^{-1} is shown (by taking $\mu \approx 1$ eV, $\varepsilon_1 \approx 10^{-4}$ eV and

temperature $T = 200$ K, and the amplitude is multiplied by a very large factor to get clear oscillation (i.e an oscillation with observable amplitude), since the oscillation is too small to observe and this graph looks that of Bismuth [3].

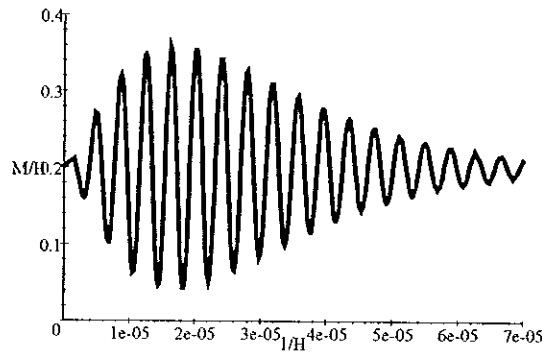
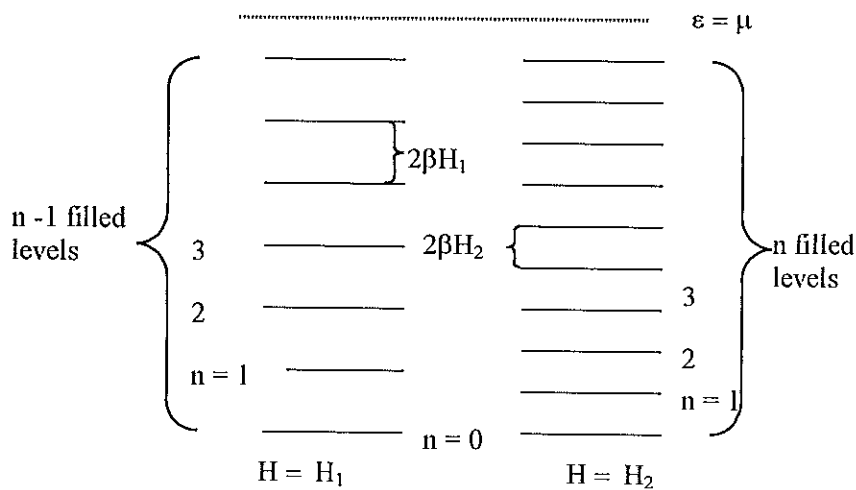


Fig. 3.1 Theoretical plot for M^{osl}/H versus $1/H$. Significant amplitude range is seen clearly from the graph.



1. Fig 3.2 Landau levels occupation scheme; states with n and $n - 1$ filled levels below the fermi level μ are essentially the same for very large n

In section 3.2.1 we mentioned that at low temperature not only the magnetization, but almost all kinetic properties depending on the density of state at the Fermi level μ oscillate as the function of H . In Fig.3.2, the levels below μ are filled and those above μ are empty.

Since $\mu \gg 2\beta H$, the number n of occupied levels is very large. When H is increased slightly from $H = H_2$ to $H = H_1$ such that the level separation will increase from $2\beta H_2$ to $2\beta H_1$, and if this results in crossing the fermi level $\varepsilon = \mu$ from below by the upper most filled level, the resulting distribution of levels is similar to the original one except that the number of filled levels below $\varepsilon = \mu$ is now $n - 1$ instead of n . Since n is very large, this difference is essentially negligible, so that one expects the new state to be equivalent to the original one.

Hence, $\varepsilon_{n,H_2}(p_z) = 2\beta H_2 \left(n + \frac{1}{2}\right) + \varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right)$ and $\varepsilon_{n-1,H_1}(p_z) = 2\beta H_1 \left((n-1) + \frac{1}{2}\right) + \varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right)$, since due to the increase of H from H_2 to H_1 the number of filled levels below $\varepsilon = \mu$ is shifted from n to $n - 1$, the increase in the energy levels due to the increase in H is compensated by the lowering of the filled quantum number, so that $\varepsilon_{n,H_2}(p_z) = \varepsilon_{n-1,H_1}(p_z)$, so for very large n , $n \approx n - 1$, and we can say $\varepsilon_{n,H_2}(p_z) = \varepsilon_{n,H_1}(p_z) = \varepsilon_{n,H_2+(H_1-H_2)}(p_z) = \varepsilon_{n,H_2+\Delta H}(p_z)$, and hence

$$\varepsilon_{n,H_2}(p_z) = \varepsilon_{n,H_2+\Delta H}(p_z).$$

Thus, we can say that $\varepsilon_{n,H}(p_z)$ is periodic with a periodicity $\Delta H = H_1 - H_2$. Similarly, $\Omega_{n,H}(p_z)$ is periodic with a periodicity $\Delta H = H_1 - H_2$ so that

$$\Omega_{n,H_2}(p_z) = \Omega_{n,H_2+\Delta H}(p_z).$$

Therefore, magnetization, being function of $\frac{1}{H}$, will also be periodic with periodicity of $\Delta\left(\frac{1}{H}\right) = \frac{1}{H_2} - \frac{1}{H_1}$. This shows the periodic dependence of magnetization on $\frac{1}{H}$.

3.4 Consideration of the Fermi Liquid Effect

We know that the change in the energy of a quasi particle in presence of external fields is $\delta\varepsilon(\mathbf{p}, \mathbf{r}, \boldsymbol{\sigma}, t) = e\varphi(\mathbf{r}, t) + Tr_{\boldsymbol{\sigma}'} \int f(\mathbf{p}, \hat{\boldsymbol{\sigma}}; \mathbf{p}', \hat{\boldsymbol{\sigma}}') \delta n(\mathbf{p}', \mathbf{r}, \hat{\boldsymbol{\sigma}}', t) \frac{d^3\mathbf{p}'}{(2\pi\hbar)^3}$. But in presence of only static magnetic field $\mathbf{H} = (0, 0, H)$, (i.e., no external electric field), there is no time and position dependence. The system is in equilibrium, with energy of each quasi-particle being $\varepsilon = \varepsilon(\mathbf{p}, \boldsymbol{\sigma})$ instead of $\varepsilon(\mathbf{p}, \mathbf{r}, \boldsymbol{\sigma}, t)$, and the position and/or time dependent Coulomb term $e\varphi(\mathbf{r}, t)$ is absent, and the corresponding distribution function is $n = n(\mathbf{p}, \boldsymbol{\sigma})$. The part of the change in the energy of the quasi particle due to the change in the distribution function of the other quasi particles in presence of only a static magnetic field is $Tr_{\boldsymbol{\sigma}'} \int f(\mathbf{p}, \boldsymbol{\sigma}; \mathbf{p}', \boldsymbol{\sigma}') \delta n(\mathbf{p}', \boldsymbol{\sigma}') \frac{d^3\mathbf{p}'}{(2\pi\hbar)^3}$. The corresponding change in the energy of the quasi-particle due to the direct interaction of the static magnetic field with the spin is function only of the spin parameter $\boldsymbol{\sigma}$ and is given by $-\beta\boldsymbol{\sigma}\mathbf{H}$. As a result, the total change in the energy of the quasi-particle $\delta\varepsilon(\mathbf{p}, \boldsymbol{\sigma})$, denoted by $-\beta_1(\mathbf{p})\boldsymbol{\sigma}\mathbf{H}$, becomes $\delta\varepsilon(\mathbf{p}, \boldsymbol{\sigma}) = -\beta_1(\mathbf{p})\boldsymbol{\sigma}\mathbf{H} = -\beta\boldsymbol{\sigma}\mathbf{H} + Tr_{\boldsymbol{\sigma}'} \int f(\mathbf{p}, \boldsymbol{\sigma}; \mathbf{p}', \boldsymbol{\sigma}') \delta n(\mathbf{p}', \boldsymbol{\sigma}') \frac{d^3\mathbf{p}'}{(2\pi\hbar)^3}$. Since the variation of the distribution function $\delta n(\mathbf{p}', \boldsymbol{\sigma}')$ is due to the variation in energy $\delta\varepsilon(\mathbf{p}, \boldsymbol{\sigma}) = -\beta_1(\mathbf{p})\boldsymbol{\sigma}\mathbf{H}$,

$$\delta n(\mathbf{p}', \boldsymbol{\sigma}') = -\frac{\partial n'_o}{\partial \varepsilon'} \beta_1(\mathbf{p}') \boldsymbol{\sigma}' \mathbf{H}; \quad (3.17)$$

but $-\frac{\partial n'_o}{\partial \varepsilon'} = \delta_c(\varepsilon' - \varepsilon_F)$ and the Landau's correlation function is given by

$$f(\mathbf{p}, \boldsymbol{\sigma}; \mathbf{p}', \boldsymbol{\sigma}') = \eta(\mathbf{p}, \mathbf{p}') + \boldsymbol{\sigma}\boldsymbol{\sigma}'\zeta(\mathbf{p}, \mathbf{p}'), \quad (3.18)$$

so that $\delta\varepsilon(\mathbf{p}, \boldsymbol{\sigma})$ becomes

$$\beta_1(\mathbf{p})\boldsymbol{\sigma}\mathbf{H} = \beta\boldsymbol{\sigma}\mathbf{H} + Tr_{\boldsymbol{\sigma}'} \int [\eta(\mathbf{p}, \mathbf{p}') + \boldsymbol{\sigma}\boldsymbol{\sigma}'\zeta(\mathbf{p}, \mathbf{p}')] \frac{\partial n'_o}{\partial \varepsilon'} \beta_1(\mathbf{p}') \boldsymbol{\sigma}' \mathbf{H} \frac{d^3\mathbf{p}'}{(2\pi\hbar)^3}. \quad (3.19)$$

Eventhough the expression for $f(\mathbf{p}, \sigma; \mathbf{p}', \sigma')$ in (3.18) is valid only in isotropic medium, it is approximately valid in real metals for otherwise the second term must have been $\sigma_j \sigma'_k \zeta_{jk}(p, p')$ so that f becomes a tensor. Here, we considered only the spin dependent correlation function, though there may also be other additional terms involving the direct interaction between the magnetic moments and the spin-orbit coupling. In (3.18), $\sigma \sigma' \zeta(\mathbf{p}, \mathbf{p}')$ is exchange term arising as a result of the coulomb interaction between electrons. From section 1.6, the kinetic equation in relaxation time approximation, in the assumption that the external electric field \mathbf{E} is weak, is given by (1.26), i.e., $\frac{\partial \psi}{\partial t} + \frac{\partial \psi}{\partial \mathbf{r}} \mathbf{v} - e\mathbf{v}\mathbf{E} + \frac{\partial \psi}{\partial t_H} - \frac{\partial \psi}{\partial t} = -\frac{\psi}{\tau}$, but since there is no position and time dependent external field in general and no any external electric field, the first, the second, third and fifth terms of the left hand side of this equation vanishes and we obtain

$$\frac{\partial \psi}{\partial t_H} = \frac{e}{c} \mathbf{v} \times \mathbf{H} \frac{\partial \psi}{\partial \mathbf{p}} = -\frac{\psi}{\tau}. \quad (3.20)$$

We find the possible solution of (3.20) as follows. The change in the distribution function of the quasiparticles can be written as $\delta n(\mathbf{p}, \sigma) = -\frac{\partial n_0}{\partial \varepsilon} \psi$, comparing this with (3.17) we obtain

$$\psi = \beta_1(\mathbf{p}) \sigma H. \quad (3.21)$$

Substituting this in (3.20), we obtain $\frac{e}{c} \mathbf{v} \times \mathbf{H} \frac{\partial \beta_1(\mathbf{p})}{\partial \mathbf{p}} = -\frac{\beta_1(\mathbf{p})}{\tau}$, or

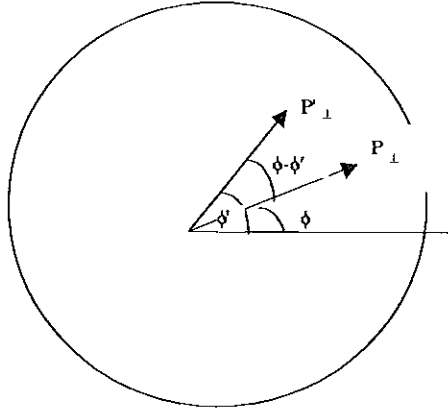
$$p_y \frac{\partial \beta_1}{\partial p_x} - p_x \frac{\partial \beta_1}{\partial p_y} = -\frac{\beta_1}{\omega_c \tau}. \quad (3.22)$$

Where $\omega_c = \frac{eH}{mc}$ is the cyclotron frequency.

For further analysis we need to construct a new coordinate system in \mathbf{p} -space labeled (ε, ϕ, p_z) as follows. From our energy spectrum $\varepsilon = \frac{p_{\perp}^2}{2m} + \varepsilon_1 \cos(\frac{\alpha p_z}{\hbar})$ we obtain

$$p_{\perp} = \sqrt{2m(\varepsilon - \varepsilon_1 \cos(\frac{\alpha p_z}{\hbar}))} = p_{\perp}(\varepsilon, p_z) \geq 0. \quad (3.23)$$

For a given p_z , our orbit is circular, hence we can use plane polar coordinate system in \mathbf{p} -space as shown in fig. 3.3



2.Fig. 3.3 Polar coordinate system in \mathbf{p} -space.

From fig. 3.3, $p_x(\varepsilon, \phi, p_z) = p_{\perp}(\varepsilon, p_z) \cos \phi$ and $p_y(\varepsilon, \phi, p_z) = p_{\perp}(\varepsilon, p_z) \sin \phi$. Through the transformation of coordinate system $(p_x, p_y, p_z) \rightarrow (\varepsilon, \phi, p_z)$, each element of the Jacobian determinant $\frac{\partial(p_x, p_y, p_z)}{\partial(\varepsilon, \phi, p_z)}$ can be calculated to obtain

$$d^3\mathbf{p} = dp_x dp_y dp_z = \frac{\partial(p_x, p_y, p_z)}{\partial(\varepsilon, \phi, p_z)} d\varepsilon d\phi dp_z = m d\varepsilon d\phi dp_z. \text{ Using these, we find}$$

$$\frac{\partial \beta_1}{\partial \phi} = \frac{\beta_1}{\omega_c \tau}.$$

Solving this differential equation, we obtain

$$\beta_1(\mathbf{p}) = \beta_1(\phi) = A e^{\frac{\phi}{\omega_c \tau}}, \quad (3.24)$$

where A is constant of integration. Hence, from (3.24) we see that the functional dependence of β_1 on \mathbf{p} is only through ϕ , so that $\delta\varepsilon(\mathbf{p}, \sigma)$ becomes

$$\beta_1(\mathbf{p})\sigma\mathbf{H} = \beta\sigma\mathbf{H} + \frac{Am\text{Tr}_{\sigma'}(\sigma'\mathbf{H})}{(2\pi\hbar)^3} \times \int [\eta(\mathbf{p}, \mathbf{p}') + \sigma\sigma'\zeta(\mathbf{p}, \mathbf{p}')] \frac{\partial n'_o}{\partial \varepsilon'} e^{\frac{\phi'}{\omega_{c\tau'}}} d\varepsilon' d\phi' dp'_z. \quad (3.25)$$

Noting that $\text{Tr}_{\sigma'}(\sigma'_i) = 0$, since σ_i is traceless for all $i = x, y$ and z , one can calculate that $\text{Tr}_{\sigma'}\{(\sigma'\mathbf{H})(\sigma\sigma')\} = 2\sigma\mathbf{H}$. Therefore, $\eta(\mathbf{p}, \mathbf{p}')$ has no contribution in (3.25) and we have $\beta_1(\mathbf{p})\sigma\mathbf{H} = \beta\sigma\mathbf{H} + 2\sigma\mathbf{H} \frac{Am}{(2\pi\hbar)^3} \int \zeta(\mathbf{p}, \mathbf{p}') \frac{\partial n'_o}{\partial \varepsilon'} e^{\frac{\phi'}{\omega_{c\tau'}}} d\varepsilon' d\phi' dp'_z$ or one can write

$$\beta_1 = \beta + \frac{2Am}{(2\pi\hbar)^3} \int \zeta(\varepsilon, \phi, p_z; \varepsilon', \phi', p'_z) \frac{\partial n'_o}{\partial \varepsilon'} e^{\frac{\phi'}{\omega_{c\tau'}}} d\varepsilon' d\phi' dp'_z,$$

which after integrating by replacing $\frac{\partial n'_o}{\partial \varepsilon'}$ by delta function about μ for the ε' integration we get $\beta_1 = \beta - \frac{2Am}{(2\pi\hbar)^3} \int_0^{\frac{2\pi\hbar}{a}} \int_0^{2\pi} \zeta(\varepsilon, \phi, p_z; \mu, \phi', p'_z) e^{\frac{\phi'}{\omega_{c\tau_F}}} d\phi' dp'_z$.

From the form of our energy spectrum one expects $\zeta(\mathbf{p}, \mathbf{p}')$ to be of the form [5, 6]

$$\zeta(\mathbf{p}, \mathbf{p}') = \alpha \frac{\mathbf{p}_\perp \mathbf{p}'_\perp}{P_F^2} + \gamma \frac{\mathbf{p}_\perp \mathbf{p}'_\perp p_z p'_z}{P_F^4}.$$

As can easily be observed from fig.3.3, $\mathbf{p}_\perp \mathbf{p}'_\perp = p_\perp p'_\perp \cos(\phi' - \phi)$, and using the corresponding expressions for p_\perp and p'_\perp , for $\varepsilon' = \varepsilon_F$, the correlation function ζ may be expressed as

$$\begin{aligned} \zeta &= \frac{2m\alpha}{P_F^2} \left[\varepsilon - \varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right) \right]^{\frac{1}{2}} \left[\mu - \varepsilon_1 \cos\left(\frac{ap'_z}{\hbar}\right) \right]^{\frac{1}{2}} \cos(\phi' - \phi) \\ &+ \frac{2m\gamma}{P_F^4} \left[\varepsilon - \varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right) \right]^{\frac{1}{2}} \left[\mu - \varepsilon_1 \cos\left(\frac{ap'_z}{\hbar}\right) \right]^{\frac{1}{2}} p_z p'_z \cos(\phi' - \phi) \end{aligned}$$

and using this result in the last expression of β_1 and integrating, we get

$$\beta_1 = \beta - \frac{4Am^2}{(2\pi\hbar)^3 P_F^2} \left[\varepsilon - \varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right) \right]^{\frac{1}{2}} I_1 \left(\alpha I_2 + \gamma \frac{p_z}{P_F^2} I_3 \right).$$

The integrals I_1, I_2 and I_3 are evaluated below:

$$I_1 = \int_0^{2\pi} \cos(\phi' - \phi) e^{\frac{\phi'}{\omega_c \tau_F}} d\phi' = \omega_c \tau_F (\cos \phi - \omega_c \tau_F \sin \phi) \frac{e^{\frac{2\pi}{\omega_c \tau_F}} - 1}{1 + \omega_c^2 \tau_F^2},$$

and using the fact that $\mu \gg \varepsilon_1$ in the p'_z integration it follows for I_2

$$I_2 = \int_0^{\frac{2\pi\hbar}{a}} \left[\mu - \varepsilon_1 \cos\left(\frac{ap'_z}{\hbar}\right) \right]^{\frac{1}{2}} dp'_z = \frac{2\pi\hbar}{a} \mu^{\frac{1}{2}},$$

and similarly for I_3

$$I_3 = \int_0^{\frac{2\pi\hbar}{a}} \left[\mu - \varepsilon_1 \cos\left(\frac{ap'_z}{\hbar}\right) \right]^{\frac{1}{2}} p'_z dp'_z \approx \frac{1}{2} \left(\frac{2\pi\hbar}{a} \right)^2 \mu^{\frac{1}{2}}.$$

Substituting these in the expression for β_1 , we obtain

$$\beta_1 = \beta - \frac{4Am^2 \mu^{\frac{1}{2}}}{a (2\pi\hbar)^2 P_F^2} \left[\mu - \varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right) \right]^{\frac{1}{2}} \frac{\left(e^{\frac{2\pi}{\omega_c \tau_F}} - 1 \right) \left(\frac{\cos \phi}{\omega_c \tau_F} - \sin \phi \right)}{\left(1 + \frac{1}{\omega_c^2 \tau_F^2} \right)} \left[\alpha + \gamma \frac{p_z}{P_F^2} \left(\frac{\pi\hbar}{a} \right) \right]$$

and noting that $\left[\varepsilon - \varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right) \right]^{\frac{1}{2}} = \frac{p_{\perp}}{(2m)^{\frac{1}{2}}}$, $\cos \phi = \frac{p_x}{p_{\perp}}$ and $\sin \phi = \frac{p_y}{p_{\perp}}$, we get

$$\beta_1 = \beta - \frac{2^{\frac{3}{2}} Am^{\frac{3}{2}} \mu^{\frac{1}{2}}}{a (2\pi\hbar)^2 P_F^2} \frac{\left(e^{\frac{2\pi}{\omega_c \tau_F}} - 1 \right)}{\left(1 + \frac{1}{\omega_c^2 \tau_F^2} \right)} \left(\alpha + \frac{\pi\hbar}{a} \frac{\gamma}{P_F^2} p_z \right) \left(\frac{p_x}{\omega_c \tau_F} - p_y \right).$$

Letting $k_1 = \frac{2^{\frac{3}{2}} Am^{\frac{3}{2}} \mu^{\frac{1}{2}}}{a (2\pi\hbar)^2 P_F^2} \frac{\left(e^{\frac{2\pi}{\omega_c \tau_F}} - 1 \right)}{\left(1 + \frac{1}{\omega_c^2 \tau_F^2} \right)} = \text{const}$ and $k_2 = \frac{\pi\hbar}{a} \frac{\gamma}{P_F^2}$ as another const, we can

write

$$\beta_1(\mathbf{p}) = \beta - \Theta(\mathbf{p}), \text{ where } \Theta(\mathbf{p}) = k_1 \left(\alpha + k_2 p_z \right) \left(\frac{p_x}{\omega_c \tau_F} - p_y \right). \quad (3.26)$$

We know that $\beta = \frac{e\hbar}{2mc}$, correspondingly, we can define $\beta_1(\mathbf{p})$ as

$$\beta_1(\mathbf{p}) = \frac{e\hbar}{2m_1(\mathbf{p})c}, \quad (3.27)$$

so that with (3.26) we get $\frac{e\hbar}{2m_1(\mathbf{p})c} = \frac{e\hbar}{2mc} - \Theta(\mathbf{p})$. Hence we have the following expression for the mass to inter (3.15)

$$m_1(\mathbf{p}) = \frac{m}{1 - \frac{2c}{e\hbar}m\Theta(\mathbf{p})}. \quad (3.28)$$

Therefore, in all the proceeding equations, fermi-liquid effect is said to be included if we substitute $\beta_1(p) = \frac{e\hbar}{2m_1(\mathbf{p})c}$ for β or $m_1(\mathbf{p}) = \frac{m}{1 - \frac{2c}{e\hbar}m\Theta(\mathbf{p})}$ for m . Remember that β or m is the one that came about through $\beta\hat{\sigma}\mathbf{H}$, so that one should not be confused with the ones substituted for β^* and m^* after the energy spectrum of the layered conductor is used.

Therefore the energy spectrum obtained for layered conductors in a static magnetic field $\mathbf{H} = (0, 0, H)$ is the sum of two main parts, one $\frac{p_1^2}{2m}$ which through semi classical quantization of levels became $2\beta^*H \left(n + \frac{1}{2}\right)$ and the second being $\varepsilon_1 \cos\left(\frac{ap_z}{\hbar}\right)$ identifies it from other energy spectrums in that there are one maxima and one minima for each Brillouin zone which finally made the oscillation of magnetization to be the superposition of two oscillations with distinct periods, and amplitude of very small magnitude (of the order of $10^{-10} \text{ A m}^{-1}$).

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