# Lecture note on Solid State Physics
# de Haas-van Alphen effect

Masatsugu Suzuki and Itsuko S. Suzuki
State University of New York at Binghamton
Binghamton, New York 13902-6000
(April 26, 2006)

**ABSTRACT**

Here the physics on the de Haas-van Alphen (dHvA) effect is presented. There have been many lecture notes (in Web sites) on the dHvA effect. Many of them have been written by theorists who have no experience on the measurement of the dHvA effect. One of the authors (M.S.) has studied the frequency mixing effect (dHvA) and the static skin effect (Shubnikov-de Haas effect) of bismuth (Bi) as a part of his Ph.D. Thesis (Physics) (University of Tokyo, 1977) under the instruction of Prof. Sei-ichi Tanuma (Ph.D. advisor). Around 1974, Prof. David Shoenberg (the late) visited the University of Tokyo and gave an excellent talk on the dHvA effect of copper at the Physics Colloquium (Prof Ryogo Kubo was also present). When he explained the dHvA period related to the dog's bone, he pronounced it in Japanese, "inu no hone." His talk was very impressive and greatly entertained the audience of the Physics Department. Before his talk, Prof. Shoenberg also visited the Institute of Solid State Physics at the University of Tokyo. At that time, M.S. measured the dHvA effect of copper to examine the possibility of the zone oscillation effect. Prof. Shoenberg gave invaluable suggestions to M.S. on the experiment (unfortunately this experiment has failed) and greatly encouraged M.S. to continue to do the dHvA experiments.

This lecture note is written based on the experience of M.S. during his Ph.D. work on the dHvA effect. Note that the pioneering works on the dHvA of Bi were done by Prof. Shoenberg [Proc. Roy. Soc. A **156**, 687 (1936), Proc. Roy. Soc. A **156**, 701 (1936), Proc. Roy. Soc. A **170**, 341 (1936)]. Numerical calculations (although they are very simple calculations) are made by Mathematica 5.2. For convenience, one program is also given in the Appendix.

Notations:

$\hbar$: Planck constant
$c$: velocity of the light
$-e$: charge of electron
$m_0$: mass of free electron
$m_c$: cyclotron mass
$m$: mass of electron (in theory)
$\omega_c$: cyclotron frequency ($\omega_c = eB/(m_c c)$)
$\mu_B$ Bohr magneton ($\mu_B = e\hbar/(2m_0 c)$)
$\Phi_0$: quantum fluxoid ($\Phi_0 = 2\pi\hbar c/2e = 2.0678\times10^{-7}$ Gauss cm$^2$)
$B$: magnetic field
$l$: magnetic length ($l = \sqrt{c\hbar/eB}$)
T: Tesla (1 T = $10^4$ Oe)
Oe unit of the magnetic field (= Gauss)
$\varepsilon_F$: the Fermi energy
$S_e$: extremal cross-sectional area of the Fermi surface in a plane normal to the magnetic field.

## Contents



## 1. Introduction

The de Haas-van Alphen (dHvA) effect is an oscillatory variation of the diamagnetic susceptibility as a function of a magnetic field strength (*B*). The method provides details of the extremal areas of a Fermi surface. The first experimental observation of this behavior was made by de Haas and van Alphen (1930). They have measured a magnetization *M* of semimetal bismuth (Bi) as a function of the magnetic field (*B*) in high fields at 14.2 K and found that the magnetic susceptibility *M*/*B* is a periodic function of the reciprocal of the magnetic field (1/*B*). This phenomenon is observed only at low temperatures and high magnetic fields. Similar oscillatory behavior has been also observed in magnetoresistance (so called the Shubnikov-de Haas effect).

The dHvA phenomenon was explained by Landau[1] 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 mechanics. The phenomenon became of even greater interest and importance when Onsager[2] pointed out that the change in $1/B$ through a single period of oscillation was determined by the remarkably simple relation,

$$P = \frac{1}{F} = \Delta(\frac{1}{B}) = \frac{2\pi e}{\hbar c}\frac{1}{S_e}, \qquad (1)$$

where $P$ is the period (Gauss$^{-1}$) of the dHvA oscillation in $1/B$, $F$ is the dHvA frequency (Gauss), and $S_e$ is any extremal cross-sectional area of the Fermi surface in a plane normal to the magnetic field. If the $z$ axis is taken along the magnetic field, then the are of a Fermi surface cross section at height $k_z$ is $S(k_z)$ and the extremal areas $S_e$ are the values of $S(k_z)$ at the $k_z$ where $dS(k_z)/dk_z = 0$. Thus maximum and minimum cross sections are among the extremal ones. Since altering the magnetic field direction brings different extremal areas into play, all extremal areas of the Fermi surface can be mapped out. When there are two extremal cross-sectional area of the Fermi surface in a plane normal to the magnetic field and these two periods are nearly equal, a beat phenomenon of the two periods will be observed. Each period must be disentangled through the analysis of the Fourier transform.

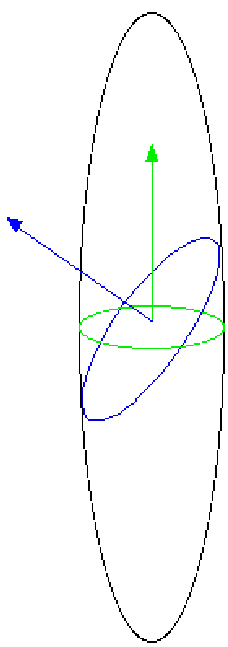


**Fig.1** Fermi surface of the hole pocket for Bi. The magnetic field (denoted by arrows) is in the *YZ* plane.

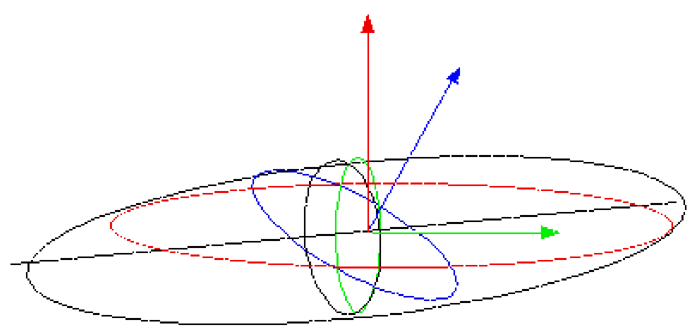


**Fig.2** Fermi surface of the electron (*a*) pocket for Bi. The major axis of the ellipsoid is tilted by 6.5º from the bisectrix axis.

Experimentally the value of $S_e$ (cm$^{-2}$) can be determined from more convenient form

$$S_e = \frac{2\pi e}{\hbar c P} = \frac{2\pi^2}{\Phi_0}\frac{1}{P} = 9.54592\times 10^7 \text{ (Gauss}^{-1}\text{ cm}^{-2})/P(\text{Gauss}^{-1})\ [\text{cm}^{-2}] \qquad (2)$$

where $P$ is in unit of Gauss$^{-1}$ and $\Phi_0$ (= $2\pi\hbar c/2e = 2.0678\times 10^{-7}$ Gauss cm$^2$) is the quantum fluxoid.

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

$$\varepsilon_F >> \hbar\omega_c >> k_B T . \qquad (3)$$

The first inequality means that the electron system is quantum-mechanically degenerate even though, as required by the second inequality, the magnetic field is sufficiently strong. On the other hand, the observation of dHvA oscillation is determined by

$$\frac{\Delta B}{B} \approx \frac{\hbar\omega_c}{\varepsilon_F} \approx 10^{-4} . \qquad (4)$$

That is, for the observation of oscillations, the fluctuations $\Delta B$ in an magnetic field should be small and the electron density should not be too high because the period depends on the ratio $\hbar\omega_c/\varepsilon_F$ .

## 2. Fermi surface of Bi[3-10]

### 2.1 Energy dispersion relation

Bismuth is a typical semimetal. The model of the band structure of Bi consists of a set of three equivalent electron ellipsoids at the $L$ point and a single hole ellipsoid at the $T$ point (see the Brillouin zone in Sec 2.2). In one of the electron ellipsoids ($a$-pocket), the energy $E$ is related to the momentum $\boldsymbol{p}$ in the absence of a magnetic field by

$$E(1+\frac{E}{E_G}) = \frac{1}{2m_0}\mathbf{p}\cdot\mathbf{m}^{*-1}\cdot\mathbf{p} , \qquad (5)$$

(Lax model[5] or ellipsoidal non-parabolic model) where $E_G$ is the energy gap to the next lower band and $\boldsymbol{m}^*$ is the effective mass tensor in units of the free electron mass $m_0$. The effective mass tensor $\boldsymbol{m}_a^*$ is of the form

$$\mathbf{m}_a^* = \begin{pmatrix} m_1 & 0 & 0 \\ 0 & m_2 & m_4 \\ 0 & m_4 & m_3 \end{pmatrix}, \qquad (6)$$

where 1, 2, and 3 refer to the binary ($X$), the bisectrix ($Y$), and the trigonal ($Z$) axes, respectively. The other two electron ellipsoids ($b$ and $c$ pockets) are obtained by rotations of ±120º about the trigonal axis, respectively. The effective mass tensors $\boldsymbol{m}_b^*$ for the b pocket and $\boldsymbol{m}_c^*$ for the c pocket are given by

$$\mathbf{m}_{b,c}^* = \begin{pmatrix} \frac{m_1+3m_2}{4} & \pm\frac{\sqrt{3}(m_1-m_2)}{4} & \pm\frac{\sqrt{3}m_4}{2} \\ \pm\frac{\sqrt{3}(m_1-m_2)}{4} & \frac{3m_1+m_2}{4} & \frac{-m_4}{2} \\ \pm\frac{\sqrt{3}m_4}{2} & \frac{-m_4}{2} & m_3 \end{pmatrix}. \qquad (7)$$

For the holes, the energy momentum relationship in the absence of a magnetic field is taken to be

$$E_0 - E = \frac{1}{2m_0}\mathbf{p}\cdot\mathbf{M}^{*-1}\cdot\mathbf{p}\,, \tag{8}$$

where $E_0$ is the energy of the top of the hole band relative to the bottom of the electron band and the effective mass tensor $\boldsymbol{M}^*$ for the hole pocket is

$$\mathbf{M}^* = \begin{pmatrix} M & 0 & 0 \\ 0 & M_1 & 0 \\ 0 & 0 & M_3 \end{pmatrix}. \tag{9}$$

The Fermi surface consists of one hole ellipsoid of revolution and three electron ellipsoids. One electron ellipsoid has its major axis tilted by a small positive angle (= 6.5°) from the bisectrix direction.

**Table I** Bi band parameters used by Takano and Kawamura[8]

| Mass parameter | $m_1$ | $m_2$ | $m_3$ | $m_4$ | $M_1$ | $M_3$ |
|---|---|---|---|---|---|---|
| At Fermi level | 0.0071 | 1.50 | 0.0301 | 0.170 | 0.067 | 0.76 |
| At the band edge | 0.0016 | 0.342 | 0.0068 | 0.038 | 0.048 | 0.54 |

| | |
|---|---|
| Carrier density ($H=0$) | $N=2.85\times10^{17}$ cm$^{-3}$ |
| Fermi energy ($H=0$) | $E_F=25.4$ meV |
| Overlap energy ($H=0$) | $E_0=37.6$ meV |
| Band gap | $E_g=15$ meV[27] |
| | $E_{gh}=60$ meV[16] |

| Spin-splitting factor $\gamma$[12] | Electrons A | Holes |
|---|---|---|
| $H$//binary axis | 0.356 | 0.14 |
| $H$//trigonal axis | 0.59 | 1.94 |

## 2.2 Brillouin zone and Fermi surface of Bi

The Brillouin zone and the Fermi surface of Bi are shown here.

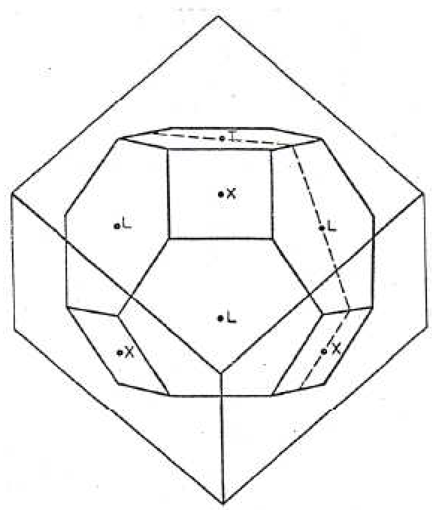



**Fig.3** Brillouin zone of bismuth[3-10]

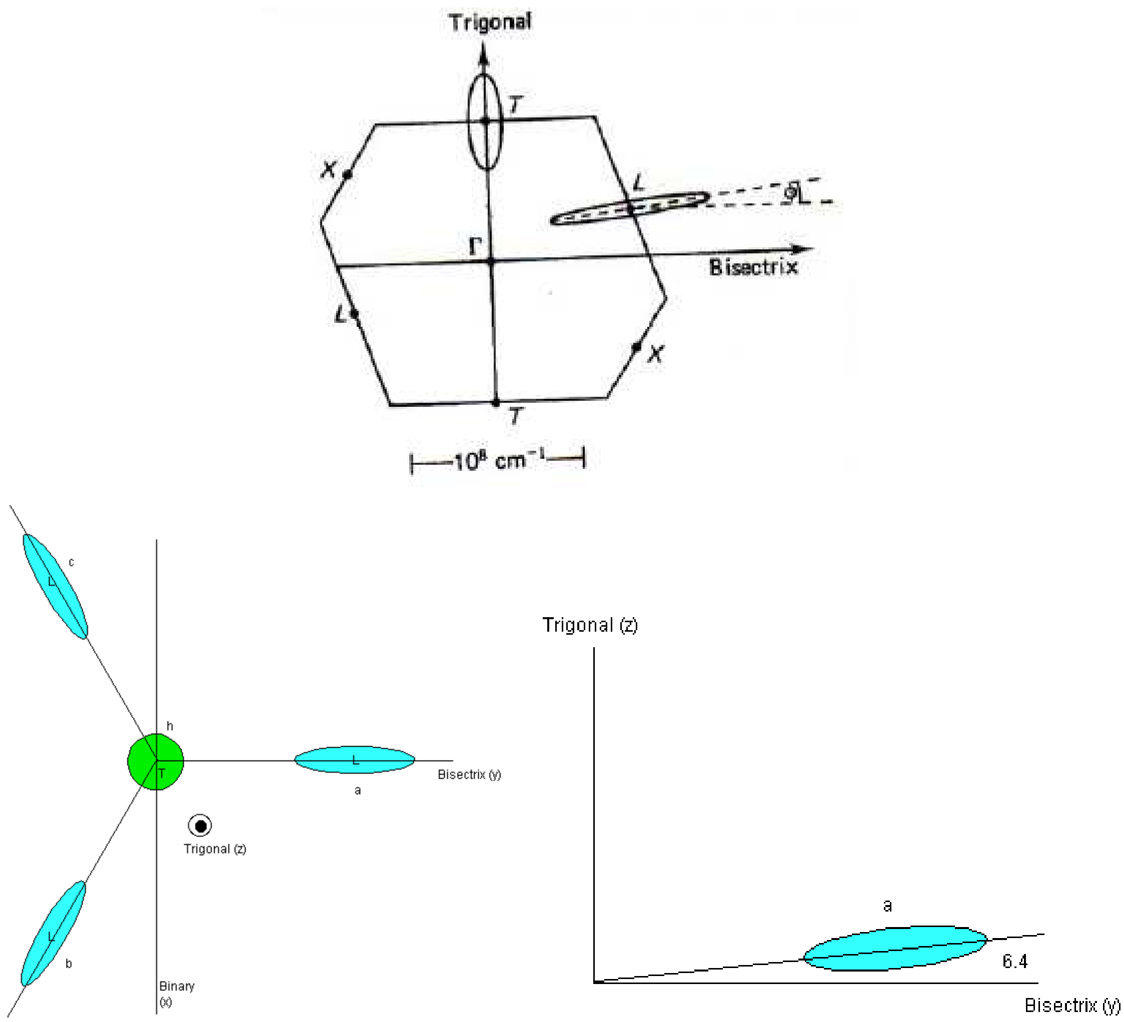



**Fig.4** Fermi surface of bismuth: binary axis ($X$), bisectrix ($Y$), and trigonal ($Z$). $a$, $b$, $c$ are the electron pocket (Fermi surfaces) and $h$ is the hole pocket.

## 3. Techniques for the measurement of dHvA

There are two major techniques to measure the dHvA oscillations: (1) field modulation method using a lock-in amplifier. (2) torque method. Because of the Fermi surface in Bi is so small, the dHvA effect can be observed in quite small fields as low as 100 Oe at 0.3 K and at fairly high temperatures up to 20 or 30 K at fields of a few kOe). It is in fact the metal in which the dHvA effect was first discovered and have probably been more studied ever since than any other metal.

### 3.1 Field-modulation method

The system consists of a detecting coil, a compensation coil, and a filed modulation coil. The static magnetic field $B$ (superconducting magnet or ion core magnet) is modulated by a small AC field $h_0\cos\omega t$ ($\omega$ is a angular frequency) generated by the field modulation coil. The direction of the AC filed is parallel to that of a static magnetic field $B$. The voltage induced in the pick-up coil is given by

$$v \propto \omega\{h\frac{\partial M}{\partial h}\sin(\omega t) + \frac{1}{2}h^2\sin(2\omega t)\frac{\partial^2 M}{\partial h^2} + ...\}, \qquad (10)$$

where $h << B$. The signal obtained from the pick-up coil is phase sensitively detected at the first harmonic or second harmonic modes with a lock-in amplifier. The DC signal is proportional to $\omega h\frac{\partial M}{\partial h}$ for the first-harmonic mode and $\omega h^2\frac{\partial^2 M}{\partial h^2}$ for the second-harmonic mode. These signals are periodic in $1/B$. The Fourier analysis leads to the dHvA frequency $F$ (or the dHvA period $P = 1/F$).

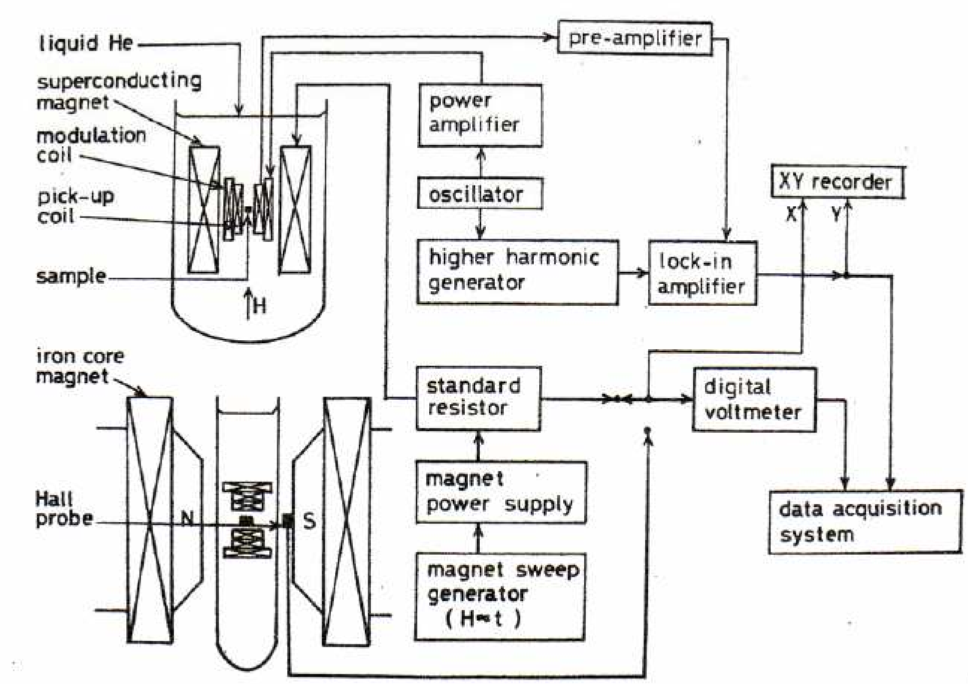



**Fig.5** The block diagram of the apparatus for the measurement of the dHvA effect by means of the field modulation method.[10]

### 3.2 Torque method

When an external magnetic field is applied to the sample, there is a torque on the sample, given $M_{\perp}BV$, where $M_{\perp}$ is the component of $\boldsymbol{M}$ perpendicular to $\boldsymbol{B}$ and $V$ is the volume. Using this method, the absolute value of the magnetization can be exactly determined. Note that the torque is equal to zero when the direction of the magnetic filed is parallel to the symmetric direction of the sample.

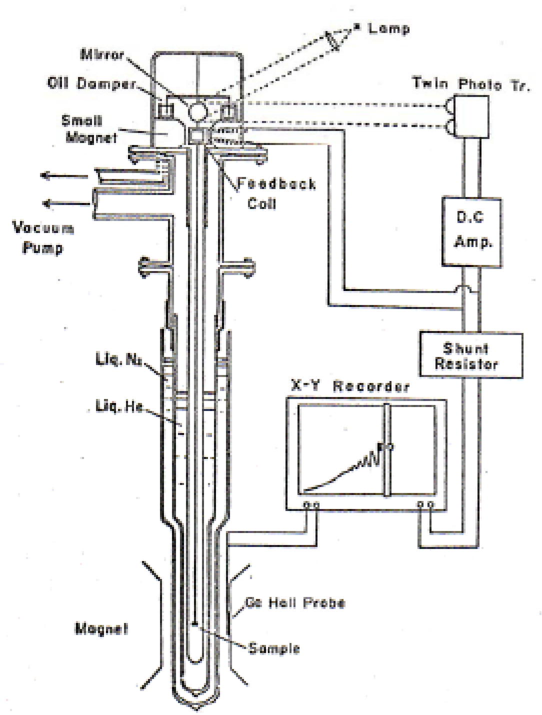



**Fig.6** The block diagram of the apparatus for measuring the dHvA effect by Torque de Haas method.[9]

## 4. Results of dHvA effect in Bi

### 4.1 Result from the modulation method (Suzuki[9])

We show typical examples of the dHvA effect in Bi and the Fourier spectra for the dH vH periods.

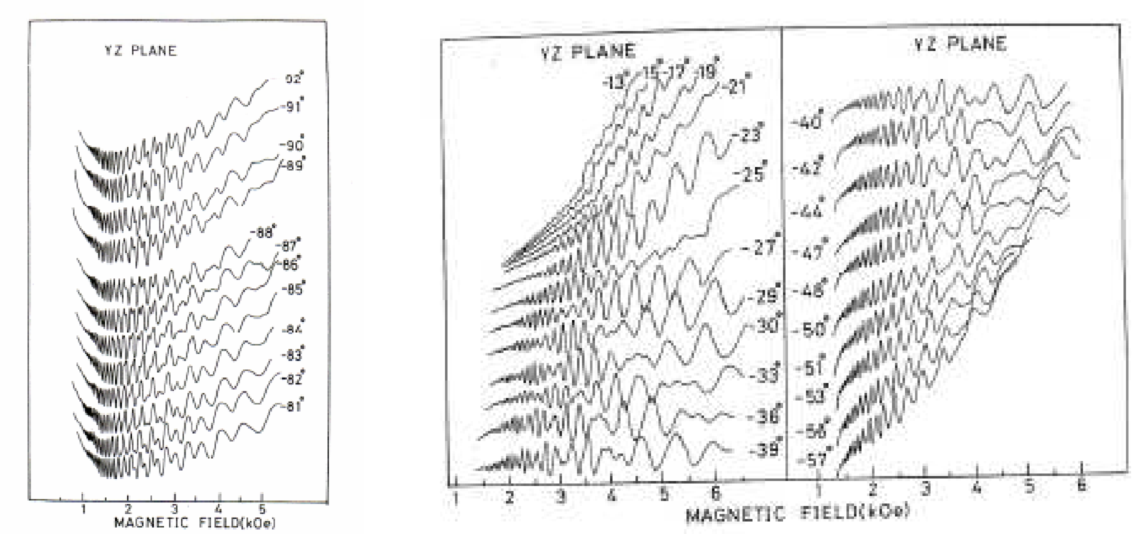



**Fig.7** The dHvA effect of Bi in the YZ plane. $T$ = 1.5 K. This signal corresponds to the first harmonics ($\partial M / \partial h$).

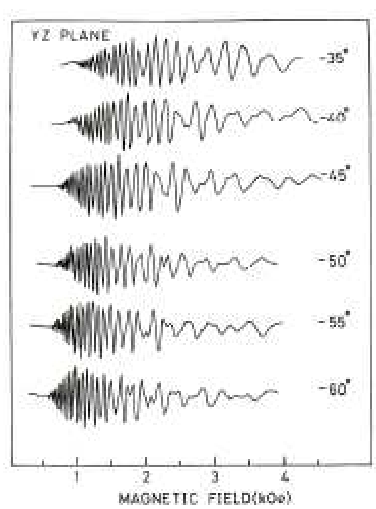



**Fig.8** The dHvA effect of Bi in the YZ plane. $T$ = 1.5 K. The signal corresponds to the second harmonics ($\partial^2 M/\partial h^2$).

## 4.2 Result of torque de Haas (Suzuki[9])

We show typical examples of the torque de Haas in Bi.

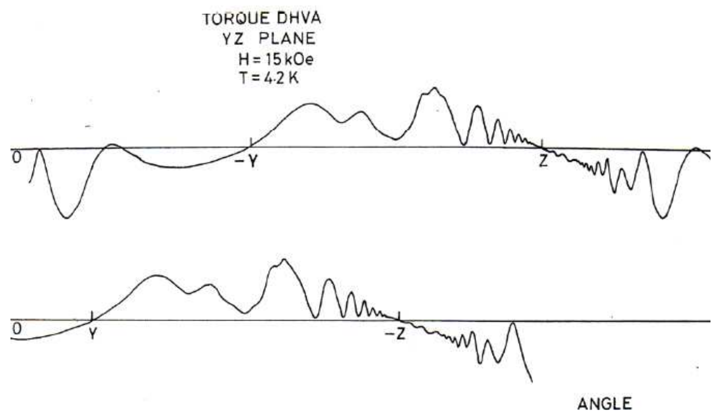



**Fig.9** Angular dependence of the torque de Has in the *YZ* plane. The torque is zero at the symmetry axes (*Y* and *Z*). $B$ = 15 kOe. $T$ = 4.2 K.

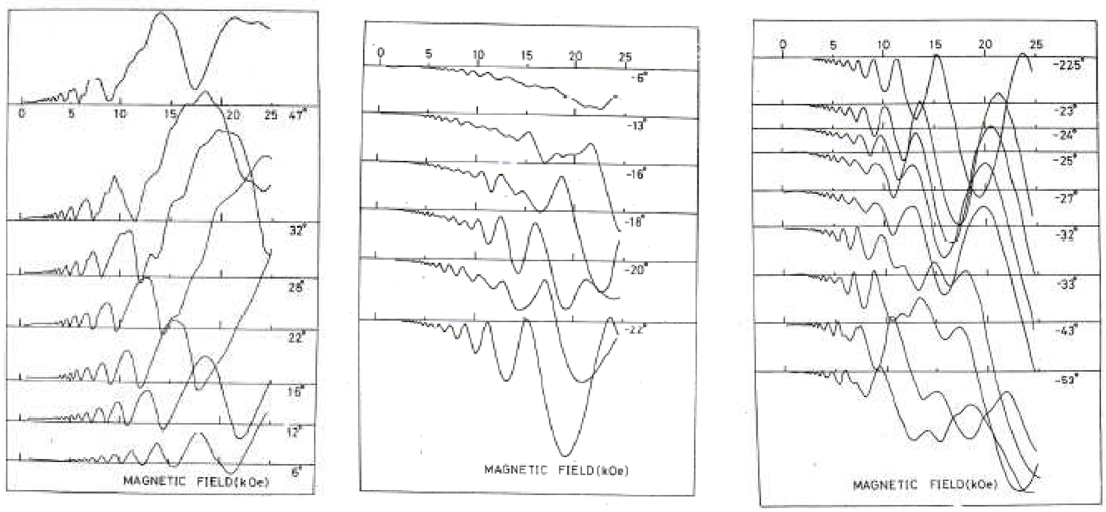



**Fig.10** The torque de Haas in the YZ plane. $T$ = 1.5 K.

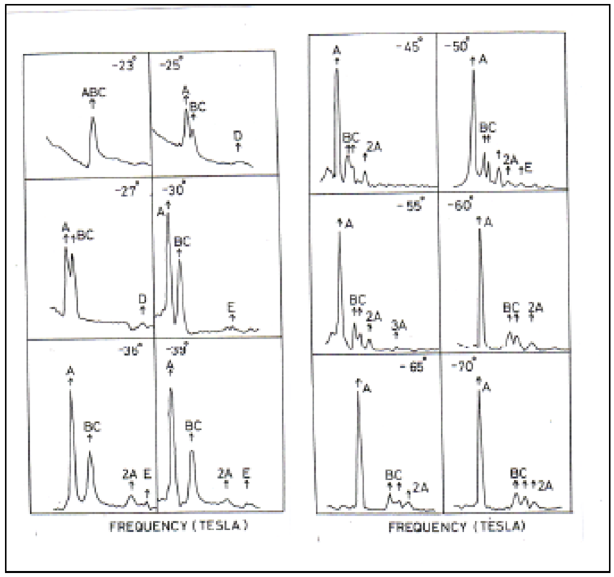



**Fig.11** The Fourier spectrum of the dHvA oscillation. The magnetic field is oriented in the YZ plane. The *Z* axis corresponds to 0º. The branches A, B, and C correspond to the *a*-, *b*-, and *c*-electron pockets, respectively. The branch E corresponds to the frequency mixing due to the quantum oscillation of the Fermi energy (see Sec.5).

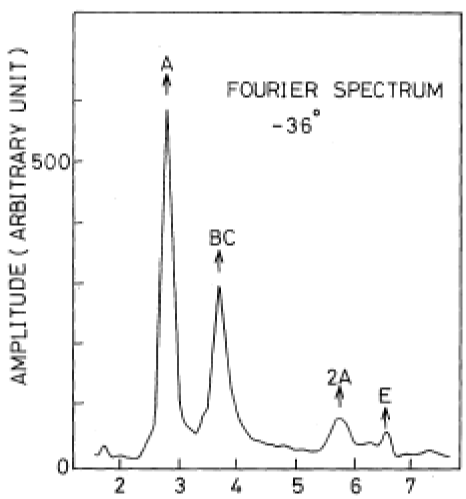



**Fig.12** The Fourier spectrum of the dHvA oscillation. The magnetic field is oriented to make -36º from the *Z* axis in the *YZ* plane. The branches A, B, and C correspond to the *a*-, *b*-, and *c*-electron pockets, respectively.

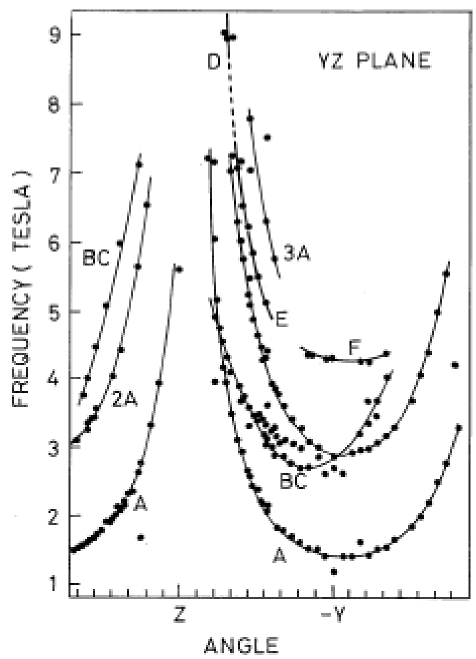



**Fig.13** The angular dependence of the dHvA frequencies in the YZ plane. The branches A, *B*, and *C* correspond to the *a*-, *b*-, and *c*-electron pockets, respectively. The dHvA frequency $F_F$ is approximately equal to $F_{3A}$, and $F_D$ and $F_E$ coincide with $F_A + F_{BC}$. Note that the *b*- and *c*- pockets separate into two branches in the range of the field angles from -48º to -70º, and this might be a result of the fact that the direction of magnetic field does not exactly lie in the *YZ* plane. Note that the frequency of $\alpha$-oscillation is denoted as $F_\alpha$ where $\alpha$ means *A, BC, D, E*, 2*A* or 3*A*.

## 4.3 Result of dHvA effect in Bi (Bhargrava[7])

**Table II** The summary of results of dHvA effect in Bi.[7]

| | Electrons | | | Holes | |
|---|---|---|---|---|---|
| Axes | Periods in $10^{-5}$ G$^{-1}$ Crystal axis | Periods in $10^{-5}$ G$^{-1}$ Ellipsoidal axis | Area in $10^{12}$ cm$^{-2}$ ellipsoidal axis | Periods in $10^{-5}$ G$^{-1}$ | Area in $10^{12}$ cm$^{-2}$ |
| 1 | 0.53±0.03 | 0.53 ±0.03 | 18.0 | 0.45 ±0.02 | 21.2 |
| | 7.20±0.05 | | | | |
| 2 | 8.30±0.05 | 8.35 ±0.05 | 1.1 | 0.45 ±0.02 | 21.2 |
| | 4.17±0.05 | | | | |
| 3 | 1.17±0.03 | 0.695±0.03 | 13.7 | 1.575±0.005 | 6.1 |

1: binary, 2: bisectrix, 3: trigonal

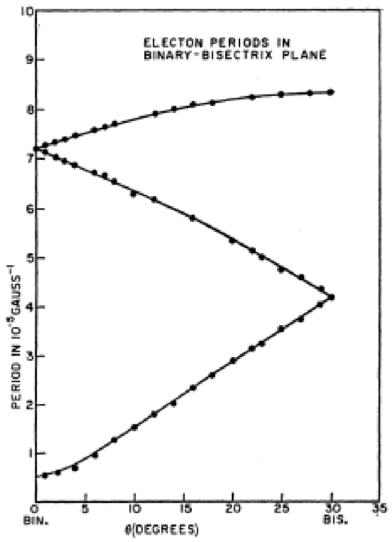



**Fig.14** The angular dependence of electron dHvA period $P$ in the XY plane for Bi. The solid line is a fit assuming an ellipsoidal Fermi surface and using the measured values of periods in the crystal axis and a tilt angle of 6.5º.[7]

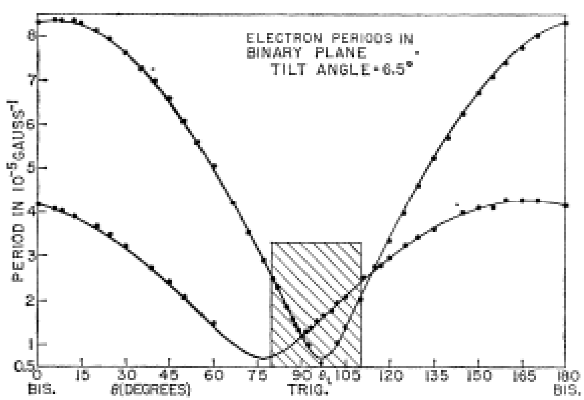



**Fig.15** The angular dependence of electron dHvA periods in the YZ plane. The tilt angle measured is 6.50±0.25º. The shaded area shows the region where electron periods were never reported. The solid line is a fit using an ellipsoidal Fermi surface.[7]

## 5. Change of Fermi energy as a function of magnetic field

The dimension of the Fermi surface of Bi is very small compared with that of ordinary metals. Therefore the quantum number of the Landau level at the Fermi energy has a small value even at a low magnetic field. The Fermi energy varies with a magnetic field in a quasi oscillatory way, since the Landau level intervals of the hole and electrons are generally different to each other. The Fermi energy is determined from the charge neutrality condition that $N_h(B) = N_e^a(B) + N_e^b(B) + N_e^c(B)$. The field dependence of the Fermi energy in Bi is shown below when $B$ is parallel to the binary, bisectrix, and trigonal axes, respectively.

We note that the dHvA frequency mixing has been observed in Bi by Suzuki et al.[10]. The Fermi energy changes at magnetic fields where the Landau level crosses the Fermi energy, so that the Fermi energy shows a pseudo periodic variation with the field. This variation is remarkable even at low magnetic field in Bi. The observed frequency mixing is due to this effect.

(a) ***B*** // the binary axis ($X$)

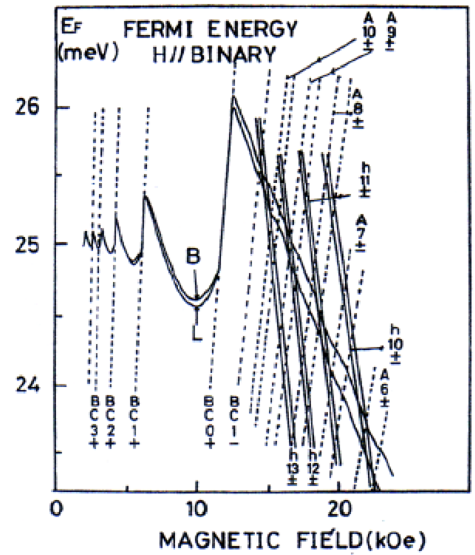



**Fig.16** The magnetic field dependence of the Fermi energy (***B*** $//X$, $T$ = 0 K). The dotted and solid lines correspond to the Landau levels of the electron and hole, respectively. The curve of $E_F$ vs $B$ exhibits kinks at the fields where the Landau levels cross the Fermi energy. *BCn*±: the Landau level of the electron *b*- and *c* pockets with the quantum number $n$ and the spin up (+) (down (-))-state. *hn*±: the Landau level of the hole pockets with the quantum number $n$ and the spin up (+) (down (-))-state. $E(n,\sigma) = \hbar\omega_c(n + \frac{1}{2} + \frac{1}{2}\nu_s\sigma)$, where $\nu_s$ is a spin-splitting factor defined in Sec.6.4, and $\sigma = \pm 1$. The expression of $E(n, \sigma)$will be discussed later. The ground Landau level is described by either Baraff[6] model (denoted B) or Lax[5] model (denoted by $L$).

(b) ***B*** // the bisectrix ($Y$)

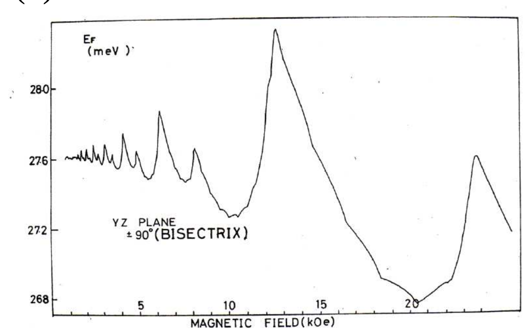



**Fig.17** The magnetic field dependence of the Fermi energy ($T$ = 0 K). Magnetic field is along the $Y$ axis (bisectrix).[9,10]

(c) ***B*** //the trigonal axis (*Z*)

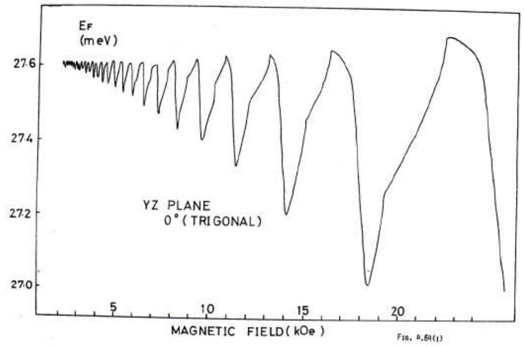



**Fig.18** The magnetic field dependence of the Fermi energy ($T$ = 0 K). Magnetic field is along the Z axis (trigonal).[9,10]

## 6. Theoretical Background[11-15]

### 6.1 The density of states: degeneracy of the Landau level

The electrons in a cubic system with side $L$ are characterized by their quantum number $\boldsymbol{k}$, with components where $\boldsymbol{k} = (k_x, k_y, k_z) = 2\pi/L\ (n_x, n_y, n_z)$ and $n_x$, $n_y$, and $n_z$ are integers. The energy of the system is given by

$$E(\mathbf{k}) = \frac{\hbar^2}{2m}\mathbf{k}^2,$$

where $m$ is the mass of electrons (we assume $m$ instead of $m_0$ in the theory, for convenience). The $\boldsymbol{k}$ space contours of constant energy are spheres and for a given $\boldsymbol{k}$ an electron has velocity given by

$$\mathbf{v}_\mathbf{k} = \frac{1}{\hbar}\nabla_\mathbf{k} E(\mathbf{k}). \qquad (11)$$

What happens in a magnetic field to the distribution of orbitals in $\boldsymbol{k}$ space? When a magnetic field $B$ is applied along the $z$ axis, the electron motion in this direction is unaffected by this field, but in the ($x$, $y$) plane the Lorentz force induces a circular motion of the electrons. The Lorentz force causes a representative point in $\boldsymbol{k}$ space to rotate in the ($k_x$, $k_y$) plane with frequency $\omega_c = eB/mc$ (we use this notation in this Section) where $-e$ is the charge of electron. This frequency, which is known as the cyclotron frequency, is independent of $\boldsymbol{k}$, so the whole system of the representative points rotate about an axis (parallel to $\boldsymbol{B}$) through the origin of $\boldsymbol{k}$ space.

This regular periodic motion introduces a new quantization of the energy levels (Landau levels) in the ($k_x$, $k_y$) plane, corresponding to those of a harmonic oscillator with frequency $\omega_c$ and energy

$$\varepsilon_n = \hbar\omega_c(n + \frac{1}{2}) = \frac{\hbar^2}{2m}k_\perp{}^2, \qquad (12)$$

where $k_\perp$ is the magnitude of the in-plane wave vector and the quantum number $n$ takes integer values 0, 1, 2, 3,….. Each Landau ring is associated with an area of $\boldsymbol{k}$ space. The area $S_n$ is the area of the orbit $n$ with the radius $k_\perp = k_n$

$$S_n = \pi k_n{}^2 = \frac{2\pi e B}{\hbar c}(n + \frac{1}{2}). \qquad (13)$$

Thus in a magnetic field the area of the orbit in $\boldsymbol{k}$ space is quantized.

The area between two adjacent Landau rings is

$$\Delta S_n = S_{n+1} - S_n = \frac{2\pi eB}{\hbar c} = \frac{2\pi}{l^2} \quad (l\text{: the magnetic length}), \tag{14}$$

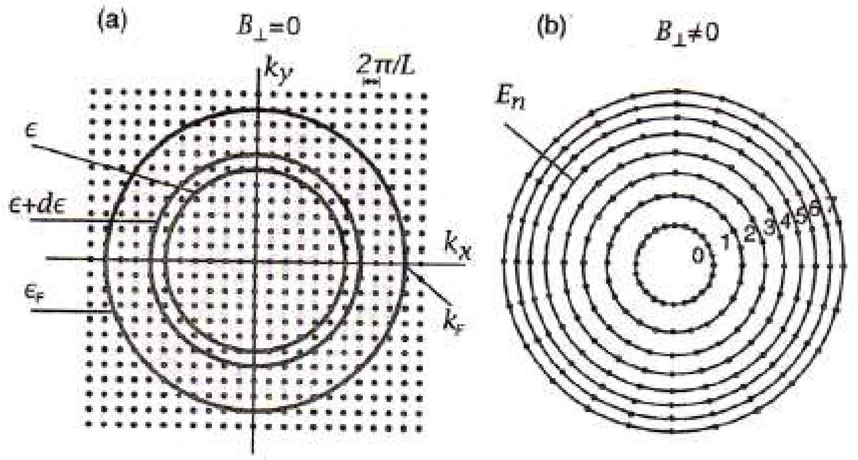



**Fig.19** Quantization scheme for free electrons. Electron states are denoted by points in the $\boldsymbol{k}$ space in the absence and presence of external magnetic field $\boldsymbol{B}$. The states on each circle are degenerate. (a) When $\boldsymbol{B}$ = 0, there is one state per area $(2\pi/L)^2$. (b) When $\boldsymbol{B} \neq 0$, the electron energy is quantized into Landau levels. Each circle represents a Landau level with energy $E_n = \hbar\omega_c(n+1/2)$.

The degeneracy of a quantum number $n$ (the number of states) is

$$D = \rho B = \frac{\Delta S_n}{\left(\frac{2\pi}{L}\right)^2} = \frac{2\pi eB}{\hbar c}\left(\frac{L}{2\pi}\right)^2 = \frac{eBL^2}{2\pi\hbar c}, \qquad \text{or} \qquad \rho = \frac{eL^2}{2\pi\hbar c}, \tag{15}$$

## 6.2 Semiclassical quantization of orbits in a magnetic field

The Onsager-Lifshitz idea[2,11] was based on a simple semi-classical treatment of how electrons move in a magnetic field, using the Bohr-Sommerfeld condition to quantize the motion. The dHvA frequency $F$ (i.e., the reciprocal of the period in $1/B$) is directly proportional to the extremal cross-section area $S$ of the Fermi surface.

The Lagrangian of the electron in the presence of electric and magnetic field is given by

$$L = \frac{1}{2}m\mathbf{v}^2 - q(\phi - \frac{1}{c}\mathbf{v}\cdot\mathbf{A}), \tag{16}$$

where $m$ and $q$ are the mass and charge of the particle.

Canonical momentum:

$$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}} = m\mathbf{v} + \frac{q}{c}\mathbf{A}. \tag{17}$$

Mechanical momentum:

$$\boldsymbol{\pi} = m\mathbf{v} = \mathbf{p} - \frac{q}{c}\mathbf{A}. \tag{18}$$

The Hamiltonian:

$$H = \mathbf{p}\cdot\mathbf{v} - L = (m\mathbf{v} + \frac{q}{c}\mathbf{A})\cdot\mathbf{v} - L = \frac{1}{2}m\mathbf{v}^2 + q\phi = \frac{1}{2m}(\mathbf{p} - \frac{q}{c}\mathbf{A})^2 + q\phi. \qquad (19)$$

The Hamiltonian formalism uses the vector potential ***A*** and the scalar potential $\phi$, and not ***E*** and ***B***, directly. The result is that the description of the particle depends on the gauge chosen.

We assume that the orbits in a magnetic field are quantized by the Bohr-Sommerfeld relation

$$\boldsymbol{\pi} = m\mathbf{v} = \hbar\mathbf{k} = \mathbf{p} - \frac{q}{c}\mathbf{A} = \mathbf{p} + \frac{e}{c}\mathbf{A}. \qquad (20)$$

$$\oint \mathbf{p}\cdot d\mathbf{r} = (n+\gamma)2\pi\hbar. \qquad (21)$$

where $q = -e$ ($e>0$) is the charge of electron, $n$ is an integer, and $\gamma$ is the phase correction: $\gamma = 1/2$ for free electron.

$$\oint \mathbf{p}\cdot d\mathbf{r} = \oint \hbar\mathbf{k}\cdot d\mathbf{r} - \frac{e}{c}\oint \mathbf{A}\cdot d\mathbf{r} = (n+\gamma)2\pi\hbar. \qquad (22)$$

The equation of motion of an electron in a magnetic field is given by

$$\hbar\frac{d\mathbf{k}}{dt} = -\frac{e}{c}\mathbf{v}\times\mathbf{B}. \qquad (23)$$

This means that the change in the vector ***k*** is normal to the direction of ***B*** and is also normal to ***v*** (normal to the energy surface). Thus ***k*** must be confined to the orbit defined by the intersection of the Fermi surface with a normal to ***B***.

Since $\mathbf{v} = (1/\hbar)\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}} = d\mathbf{r}/dt$

$$\hbar\mathbf{k} = -\frac{e}{c}(\mathbf{r} - \mathbf{r}_0)\times\mathbf{B}, \qquad (24)$$

where $\boldsymbol{r}_0$ [$=(x_0, y_0)$] is the position vector of the center of the orbit (guiding center):

$$x - x_0 = \frac{c\hbar}{eB}k_y,\; y - y_0 = -\frac{c\hbar}{eB}k_x, \qquad (25)$$

In the complex plane, we have the relation,

$$(x - x_0) + i(y - y_0) = \frac{c\hbar}{eB}e^{-i\pi/2}(k_x + ik_y). \qquad (26)$$

This means that the magnitude of the position vector $\boldsymbol{r} - \boldsymbol{r}_0 = (x - x_0, y - y_0)$ of the electron is related to that of the wave vector $\boldsymbol{k} = (k_x, k_y)$ by a scaling factor $\eta = l^2 = c\hbar/eB$. The phase of the position vector is different from that of the wave vector by $-\pi/2$ for the electron Fermi surface. $l$ is so-called magnetic length.

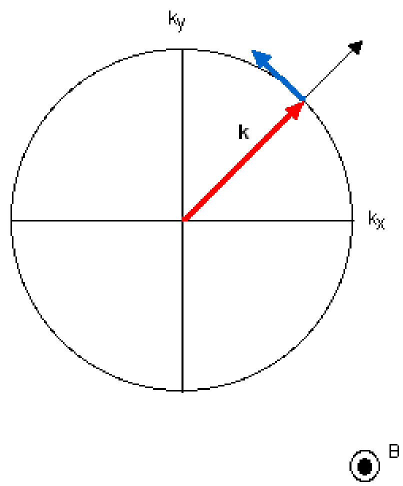



**Fig.20** The orbital motion of electron in the presence of ***B*** (***B*** is directed out of page) in the ***k***-space is similar to that in the ***r***-space but scaled by the factor $\eta$ and through $\pi/2$.[12]

Note we assume $\boldsymbol{r}_0 = 0$ in this figure.

$$\oint \hbar\mathbf{k}\cdot d\mathbf{r} = -\frac{e}{c}\oint \mathbf{r}\times\mathbf{B}\cdot d\mathbf{r} = \frac{e}{c}\mathbf{B}\cdot\oint(\mathbf{r}\times d\mathbf{r}) = \frac{e}{c}\mathbf{B}\cdot 2A\mathbf{n} = \frac{2e}{c}\Phi\,. \qquad (27)$$

where

$$\oint(\mathbf{r}\times d\mathbf{r}) = 2\ (\text{area enclosed within the orbit})\ \boldsymbol{n} \qquad (\text{geometrical result})$$

and $\Phi$ is the magnetic flux contained within the orbit in real space, $\Phi = \mathbf{B}\cdot A\mathbf{n}$.
On the other hand,

$$-\frac{e}{c}\oint \mathbf{A}\cdot d\mathbf{r} = -\frac{e}{c}\oint(\nabla\times\mathbf{A})\cdot d\mathbf{a} = -\frac{e}{c}\oint \mathbf{B}\cdot d\mathbf{a} = -\frac{e}{c}\Phi\,, \qquad (28)$$

by the Stokes theorem.
Then we have

$$\oint \mathbf{p}\cdot d\mathbf{r} = \frac{2e}{c}\Phi - \frac{e}{c}\Phi = \frac{e}{c}\Phi = (n+\gamma)2\pi\hbar\,. \qquad (29)$$

It follows that the orbit of an electron is quantized in such a way that the flux through it is

$$\Phi_n = (n+\gamma)\frac{2\pi\hbar c}{e} = 2\Phi_0(n+\gamma)\ \text{(Onsager relation)}, \qquad (30)$$

where $\Phi_0$ is a quantum fluxoid and is given by

$$\Phi_0 = \frac{2\pi\hbar c}{2e} = \frac{hc}{2e} = 2.0678\times10^{-7}\ \text{Gauss cm}^2. \qquad (31)$$

In the dHvA we need the area of the orbit in the ***k***-space. We define $S_n(\boldsymbol{r})$ as an area enclosed by the orbit in the real space ($\boldsymbol{r}$) and $S_n(\boldsymbol{k})$ as an are enclosed by the orbit in the ***k***-space. Then we have a relation

$$S_n(\mathbf{r}) = \left(\frac{c\hbar}{eB}\right)^2 S_n(\mathbf{k}) = l^2 S_n(\mathbf{k})\,. \qquad (32)$$

The quantized magnetic flux is given by

$$\Phi_n = BS_n(\mathbf{r}) = Bl^2 S_n(\mathbf{k}) = (n+\gamma)\frac{2\pi\hbar c}{e} = 2\Phi_0(n+\gamma)\,, \tag{33}$$

or

$$S_n(\mathbf{k}) = (n+\gamma)\frac{2\pi\hbar c}{e}\frac{1}{B}\frac{e^2B^2}{c^2\hbar^2} = (n+\gamma)\frac{2\pi e}{\hbar c}B\,. \tag{34}$$

Note that this equation can also be derived from the correspondence principle. The frequency for motion along a closed orbit is

$$\omega_c = \frac{eB}{m_c c}\,, \tag{35}$$

where $\omega_c$ is defined as

$$m_c = \frac{1}{2\pi}\frac{\partial S}{\partial \varepsilon}\,, \tag{36}$$

In the semiclassical limit, one should obtain equidistant levels with a separation $\Delta\varepsilon$ equal to $\hbar\omega_c$.

Hence

$$\Delta\varepsilon = \hbar\omega_c = \frac{2\pi e\hbar B}{c(\partial S/\partial\varepsilon)}\,, \tag{37}$$

or

$$\frac{\partial S}{\partial \varepsilon}\Delta\varepsilon = \Delta S = \frac{2\pi e\hbar B}{c}\,. \tag{38}$$

In the Fermi surface experiments we may be interested in the increment $\Delta B$ for which two successive orbits, $n$ and $n$+1, have the same are in the $\boldsymbol{k}$-space on the Fermi surface

$$S_n(\mathbf{k}) = S_{n+1}(\mathbf{k}) = S(\mathbf{k})$$

$$(n+\gamma)\frac{2\pi e}{\hbar c}B_n = (n+1+\gamma)\frac{2\pi e}{\hbar c}B_{n+1}\,,$$

$$\frac{S(\mathbf{k})}{B_n} = (n+\gamma)\frac{2\pi e}{\hbar c}\,,\quad \frac{S(\mathbf{k})}{B_{n+1}} = (n+1+\gamma)\frac{2\pi e}{\hbar c}\,, \tag{39}$$

or

$$S(\mathbf{k})\left(\frac{1}{B_n} - \frac{1}{B_{n+1}}\right) = \frac{2\pi e}{\hbar c}\,. \tag{40}$$

## 6.3 Quantum mechanics

### 6.3.1 Landau gauge, symmetric gauge, and gauge transformation

$$H = \frac{1}{2m}(\mathbf{p} - \frac{q}{c}\mathbf{A})^2 + q\phi = \frac{1}{2m}(\mathbf{p} + \frac{e}{c}\mathbf{A})^2 - e\phi\,. \tag{41}$$

In the presence of the magnetic field $\boldsymbol{B}$ (constant), we can choose the vector potential as

$$\mathbf{A} = \frac{1}{2}(\mathbf{B}\times\mathbf{r}) = \frac{1}{2}\begin{vmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ 0 & 0 & B \\ x & y & z \end{vmatrix} = \frac{1}{2}(-By, Bx, 0) \text{ (symmetric gauge).} \tag{42}$$

Here we define a gauge transformation between the vector potentials $\boldsymbol{A}$ and $\boldsymbol{A}$',

$$\mathbf{A}' = \mathbf{A} + \nabla\chi\,,$$

where $\chi = \frac{1}{2}Bxy$.

Since

$$\nabla\chi = \frac{1}{2}B(y, x, 0), \tag{43}$$

the new vector potential $\mathbf{A}'$ is obtained as

$$\mathbf{A}' = (0, Bx, 0) \text{ (Landau gauge).} \tag{44}$$

The corresponding gauge transformation for the wave functions,

$$\psi'(\mathbf{r}) = \exp(\frac{iq\chi}{c\hbar})\psi(\mathbf{r}) = \exp(\frac{-ieB}{2c\hbar}xy)\psi(r), \tag{45}$$

with $q = -e$ ($e>0$).

### 6.3.2 Operators in quantum mechanics

We begin by the relation

$$\hat{\boldsymbol{\pi}} = \hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}.$$

$$\begin{aligned}[\hat{\pi}_x, \hat{\pi}_y] &= [\hat{p}_x + \frac{e}{c}A_x, \hat{p}_y + \frac{e}{c}A_y] = \frac{e}{c}[\hat{p}_x, A_y] - \frac{e}{c}[\hat{p}_y, A_x] \\ &= \frac{e\hbar}{ic}\frac{\partial A_y}{\partial\hat{x}} - \frac{e\hbar}{ic}\frac{\partial A_x}{\partial\hat{y}} = \frac{e\hbar}{ic}B_z\end{aligned}, \tag{46}$$

or

$$[\hat{\pi}_x, \hat{\pi}_y] = \frac{e\hbar}{ic}B_z, \tag{47}$$

where $\frac{\partial A_y}{\partial\hat{x}} - \frac{\partial A_x}{\partial\hat{y}} = B_z$.

Similarly we have

$$[\hat{\pi}_y, \hat{\pi}_z] = \frac{e\hbar}{ic}B_x, \quad \text{and} \quad [\hat{\pi}_z, \hat{\pi}_x] = \frac{e\hbar}{ic}B_y, \tag{48}$$

Since $\boldsymbol{A}$ commute with $\hat{\mathbf{r}}$ ($\boldsymbol{A}$ is a function of $\hat{\mathbf{r}}$),

$$[\hat{x}, \hat{\pi}_x] = [\hat{x}, \hat{p}_x] = i\hbar, \quad [\hat{y}, \hat{\pi}_y] = [\hat{y}, \hat{p}_y] = i\hbar, \quad [\hat{z}, \hat{\pi}_z] = [\hat{z}, \hat{p}_z] = i\hbar.$$

$$[\hat{x}, \hat{\pi}_y] = [\hat{x}, \hat{p}_y + \frac{e}{c}A_y] = 0, \quad [\hat{y}, \hat{\pi}_x] = [\hat{y}, \hat{p}_x + \frac{e}{c}A_x] = 0, \tag{49}$$

When $\boldsymbol{B} = (0,0,B)$ or $B_z = B$,

$$[\hat{\pi}_x, \hat{\pi}_y] = \frac{e\hbar B}{ic}, \quad [\hat{\pi}_y, \hat{\pi}_z] = 0, \quad [\hat{\pi}_z, \hat{\pi}_x] = 0, \tag{50}$$

Note that

$$[\hat{\pi}_x, \hat{\pi}_y] = \frac{e\hbar^2 B}{ic\hbar} = -i\frac{\hbar^2}{\ell^2}, \tag{51}$$

where $l$ is called as a magnetic length and it is a cyclotron radius for the ground state Landau level: $\ell^2 = c\hbar/eB$

Here we define the operators $\hat{X}$ and $\hat{Y}$ for the guiding-center coordinates.

$$\hat{X} = \hat{x} - \frac{c}{eB}\hat{\pi}_y = \hat{x} - \frac{l^2}{\hbar}\hat{\pi}_y, \qquad \hat{Y} = \hat{y} + \frac{l^2}{\hbar}\hat{\pi}_x, \tag{52}$$

The commutation relation is given by

$$[\hat{X},\hat{Y}] = [\hat{x} - \frac{l^2}{\hbar}\hat{\pi}_y, \hat{y} + \frac{l^2}{\hbar}\hat{\pi}_x] = -\frac{l^2}{\hbar}[\hat{\pi}_x,\hat{x}] - \frac{l^2}{\hbar}[\hat{\pi}_y,\hat{y}] + \frac{l^4}{\hbar^2}[\hat{\pi}_x,\hat{\pi}_y] = il^2,$$

$$[\hat{\pi}_x,\hat{X}] = [\hat{\pi}_x, \hat{x} - \frac{l^2}{\hbar}\hat{\pi}_y] = [\hat{\pi}_x,\hat{x}] - [\hat{\pi}_x, \frac{l^2}{\hbar}\hat{\pi}_y] = 0,$$

$$[\hat{\pi}_x,\hat{Y}] = [\hat{\pi}_x, \hat{y} + \frac{l^2}{\hbar}\hat{\pi}_x] = [\hat{\pi}_x,\hat{y}] + [\hat{\pi}_x, \frac{l^2}{\hbar}\hat{\pi}_x] = 0. \tag{53}$$

When the uncertainties $\Delta X$ and $\Delta Y$ are defined by $(\Delta X)^2 = <\hat{X}^2>$ and $(\Delta Y)^2 = <\hat{Y}^2>$, respectively, we have the uncertainty relation,

$$(\Delta X)^2(\Delta Y)^2 \geq (1/4)\left|\left\langle[\hat{X},\hat{Y}]\right\rangle\right|^2 = (1/4)l^4, \text{ or } \quad (\Delta X)(\Delta Y) \geq (1/2)l^2.$$

The Hamiltonian $\hat{H}$ is given by

$$\hat{H} = \frac{1}{2m}(\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A})^2 = \frac{1}{2m}(\hat{\pi}_x{}^2 + \hat{\pi}_y{}^2), \tag{54}$$

We define the creation and annihilation operators,

$$\hat{a} = \frac{\ell}{\sqrt{2}\hbar}(\hat{\pi}_x - i\hat{\pi}_y), \qquad \hat{a}^+ = \frac{\ell}{\sqrt{2}\hbar}(\hat{\pi}_x + i\hat{\pi}_y), \tag{55),(56}$$

or

$$\hat{\pi}_x = \frac{\hbar}{\sqrt{2}\ell}(\hat{a} + \hat{a}^+), \qquad \hat{\pi}_y = \frac{\hbar}{i\sqrt{2}\ell}(\hat{a}^+ - \hat{a}), \tag{57}$$

$$[\hat{a},\hat{a}^+] = \frac{\ell^2}{2\hbar^2}[\hat{\pi}_x - i\hat{\pi}_y, \hat{\pi}_x + i\hat{\pi}_y] = \frac{\ell^2}{\hbar^2}i[\hat{\pi}_x,\hat{\pi}_x] = \frac{\ell^2}{\hbar^2}i(-i\frac{\hbar^2}{\ell^2}) = 1,$$

$$\hat{\pi}_x{}^2 + \hat{\pi}_y{}^2 = \frac{\hbar^2}{2\ell^2}[(\hat{a} + \hat{a}^+)^2 - (\hat{a}^+ - \hat{a})^2] = \frac{\hbar^2}{\ell^2}(\hat{a}\hat{a}^+ + \hat{a}^+\hat{a}) = \frac{\hbar^2}{\ell^2}(2\hat{a}^+\hat{a} + 1),$$

Thus we have

$$\hat{H} = \frac{\hbar^2}{m\ell^2}(\hat{a}^+\hat{a} + \frac{1}{2}) = \hbar\omega_c(\hat{a}^+\hat{a} + \frac{1}{2}), \tag{58}$$

where

$$\hbar\omega_c = \frac{\hbar^2}{m_c\ell^2} = \frac{\hbar^2}{m_c(c\hbar/eB)} = \frac{\hbar eB}{m_c c}.$$

When $\hat{a}^+\hat{a} = \hat{N}$, the Hamiltonian is described by

$$\hat{H} = \hbar\omega_c(\hat{N} + \frac{1}{2}). \tag{59}$$

We thus find the energy levels for the free electrons in a homogeneous magnetic field- also known as Landau levels.

### 6.3.3 Schrödinger equation (Landau gauge)

We consider the Hamiltonian given by

$$\hat{H} = \frac{1}{2m}[\hat{p}_x{}^2 + (\hat{p}_y + \frac{e}{c}B\hat{x})^2 + \hat{p}_z{}^2], \tag{60}$$

$$\hat{\pi}_x = \hat{p}_x, \qquad \hat{\pi}_y = \hat{p}_y + \frac{e}{c}B\hat{x}, \tag{61}$$

The guiding-center coordinates are

$$\hat{X} = \hat{x} - \frac{l^2}{\hbar}\hat{\pi}_y = \hat{x} - \frac{l^2}{\hbar}(\hat{p}_y + \frac{e}{c}B\hat{x}) = -\frac{l^2}{\hbar}\hat{p}_y, \qquad \hat{Y} = \hat{y} + \frac{l^2}{\hbar}\hat{p}_x, \tag{62}$$

The Hamiltonian $\hat{H}$ commutes with $\hat{p}_y$ and $\hat{p}_z$.

$$[\hat{H}, \hat{p}_y] = 0 \quad \text{and} \quad [\hat{H}, \hat{p}_z] = 0$$

The Hamiltonian $\hat{H}$ also commutes with $\hat{X}$ : $[\hat{H}, \hat{X}] = 0$.

$$\hat{H}\left|n, k_y, k_z\right\rangle = E_n\left|n, k_y, k_z\right\rangle$$

and

$$\hat{p}_y\left|n, k_y, k_z\right\rangle = \hbar k_y\left|n, k_y, k_z\right\rangle, \text{ and } \hat{p}_z\left|n, k_y, k_z\right\rangle = \hbar k_z\left|n, k_y, k_z\right\rangle$$

$$\left\langle y\right|\hat{p}_y\left|n, k_y, k_z\right\rangle = \hbar k_y\left\langle y\middle|n, k_y, k_z\right\rangle, \qquad \left\langle z\right|\hat{p}_y\left|n, k_y, k_z\right\rangle = \hbar k_y\left\langle y\middle|n, k_y, k_z\right\rangle$$

or

$$\frac{\hbar}{i}\frac{\partial}{\partial y}\left\langle y\middle|n, k_y, k_z\right\rangle = \hbar k_y\left\langle y\middle|n, k_y, k_z\right\rangle, \quad \frac{\hbar}{i}\frac{\partial}{\partial z}\left\langle z\middle|n, k_y, k_z\right\rangle = \hbar k_z\left\langle z\middle|n, k_y, k_z\right\rangle$$

Schrödinger equation

$$\frac{1}{2m}[(\frac{\hbar}{i}\frac{\partial}{\partial x})^2 + (\frac{\hbar}{i}\frac{\partial}{\partial y} + \frac{e}{c}Bx)^2 + (\frac{\hbar}{i}\frac{\partial}{\partial y})^2]\psi(x, y, z) = \varepsilon\psi(x, y, z), \tag{63}$$

$$\psi(x, y, z) = e^{ik_y y + ik_z z}\phi(x), \tag{64}$$

$$x = \frac{\xi}{\beta}, \quad \text{with} \quad \beta = \sqrt{\frac{m\omega_c}{\hbar}} = \sqrt{\frac{eB}{\hbar c}} = \frac{1}{\ell} \quad \text{and} \quad \omega_c = \frac{eB}{mc},$$

$$\xi_0 = \beta\frac{c\hbar k_y}{eB} = \sqrt{\frac{c\hbar}{eB}}k_y = \ell k_y.$$

We assume the periodic boundary condition along the *y* axis.

$$\psi(x, y + L_y, z) = \psi(x, y, z), \tag{65}$$

or

$$e^{ik_y L_y} = 1,$$

or

$$k_y = (2\pi / L_y)n_y \ \ (n_y\text{: integers}), \tag{66}$$

Then we have

$$.\phi''(\xi) = [(\xi - \xi_0)^2 + \frac{c}{e\hbar B}(-2mE_1 + \hbar^2 k_z{}^2)]\phi(\xi)$$

We put

$$E_1 = \hbar\omega_c(n + \frac{1}{2}) + \frac{\hbar^2 k_z{}^2}{2m} \ \ \text{(Landau level)}, \tag{67}$$

or

$$2mE_1 = \hbar^2 k_z^{\ 2} + 2m\hbar\omega_c (n+\frac{1}{2}) = \hbar^2 k_z^{\ 2} + \frac{2eB\hbar}{c}(n+\frac{1}{2}),$$

$$\phi''(\xi) = [(\xi-\xi_0)^2 - (2n+1)]\phi(\xi).$$

Finally we get a differential equation for $\phi(\xi)$.

$$\phi''(\xi) + [2n+1-(\xi-\xi_0)^2]\phi(\xi).$$

The solution of this differential equation is

$$\phi_n(\xi) = (\sqrt{\pi}\, 2^n n!)^{-1/2} e^{-\frac{(\xi-\xi_0)^2}{2}} H_n(\xi-\xi_0), \tag{68}$$

with

$$\xi_0 = \sqrt{\frac{c\hbar}{eB}} k_y = \ell k_y,$$

$$\ell = \sqrt{\frac{c\hbar}{eB}},$$

$$x_0 = \frac{\xi_0}{\beta} = \ell\xi_0 = \ell^2 k_y$$

The coordinate $x_0$ is the center of orbits. Suppose that the size of the system along the $x$ axis is $L_x$. The coordinate $x_0$ should satisfy the condition, $0<x_0<L_x$. Since the energy of the system is independent of $x_0$, this state is degenerate.

$$0 < x_0 = \frac{\xi_0}{\beta} = \ell\xi_0 = \ell^2 k_y < L_x, \tag{69}$$

or

$$\ell^2 k_y = \frac{2\pi}{L_y}\ell^2 n_y < L_x,$$

or

$$n_y < \frac{L_x L_y}{2\pi\ell^2}.$$

Thus the degeneracy is given by the number of allowed $k_y$ values for the system.

$$g = \frac{L_x L_y}{2\pi\ell^2} = \frac{A}{2\pi\ell^2} = \frac{A}{2\pi\frac{c\hbar}{eB}} = \frac{BA}{2\Phi_0} = \frac{\Phi}{2\Phi_0}, \tag{70}$$

where

$$\Phi_0 = \frac{2\pi\hbar c}{2e} = 2.0678\times 10^{-7}\ \text{Gauss cm}^2.$$

The energy dispersion is plotted as a function of $k_z$ for each Landau level with the index $n$.

$$E(n,k_z) = \hbar\omega_c(n+\frac{1}{2}) + \frac{\hbar^2 k_z^{\ 2}}{2m}. \tag{71}$$

### 6.3.4 Another method

$$\hat{H} = \frac{1}{2m}(\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A})^2 = \frac{1}{2m}[\hat{\mathbf{p}}^2 + \frac{e^2}{c^2}\mathbf{A}^2 + \frac{e}{c}(\hat{\mathbf{p}}\cdot\mathbf{A} + \mathbf{A}\cdot\hat{\mathbf{p}})],$$

$$\hat{\mathbf{p}}\cdot\mathbf{A} + \mathbf{A}\cdot\hat{\mathbf{p}} = \hat{p}_x A_x + \hat{p}_y A_y + \hat{p}_z A_z + A_x\hat{p}_x + A_y\hat{p}_y + A_z\hat{p}_z$$

$$= [\hat{p}_x, A_x] + [\hat{p}_y, A_y] + [\hat{p}_z, A_z] + 2\mathbf{A}\cdot\hat{\mathbf{p}}$$
$$= \frac{\hbar}{i}\nabla\cdot\mathbf{A} + 2\mathbf{A}\cdot\hat{\mathbf{p}}.$$

Then we have

$$\hat{H} = \frac{1}{2m}[\hat{\mathbf{p}}^2 + \frac{e^2}{c^2}\mathbf{A}^2 + \frac{e}{c}(\frac{\hbar}{i}\nabla\cdot\mathbf{A} + 2\mathbf{A}\cdot\hat{\mathbf{p}})]$$

$$= \frac{1}{2m}(\hat{\mathbf{p}}^2 + \frac{e^2}{c^2}\mathbf{A}^2 + \frac{e\hbar}{ic}\nabla\cdot\mathbf{A} + \frac{2e}{c}\mathbf{A}\cdot\hat{\mathbf{p}})$$

Since $\nabla\cdot\mathbf{A} = 0$,

$$\hat{H} = \frac{1}{2m}(\hat{\mathbf{p}}^2 + \frac{e^2}{c^2}\mathbf{A}^2 + \frac{2e}{c}\mathbf{A}\cdot\hat{\mathbf{p}}) = \frac{1}{2m}\hat{\mathbf{p}}^2 + \frac{e^2B^2}{2mc^2}\hat{x}^2 + \frac{eB}{mc}\hat{x}\hat{p}_y,$$

where

$$\ell^2 = \frac{c\hbar}{eB}, \qquad \hbar\omega_c = \frac{\hbar^2}{m\ell^2} = \frac{\hbar eB}{mc}, \qquad m\omega_c^{\ 2} = \frac{e^2B^2}{mc^2},$$

$$\hat{H} = \frac{1}{2m}\hat{\mathbf{p}}^2 + \frac{e^2B^2}{2mc^2}\hat{x}^2 + \omega_c\hat{x}\hat{p}_y = \frac{1}{2m}\hat{\mathbf{p}}^2 + \frac{m\omega_c^{\ 2}}{2}\hat{x}^2 + \omega_c\hat{x}\hat{p}_y.$$

The first and second terms of this Hamiltonian are that of the simple harmonics along the *x* axis.

This Hamiltonian $\hat{H}$ commutes with $\hat{p}_y$ and $\hat{p}_z$. Thus the wave function can be described by the form,

$$\psi(x,y,z) = \phi_n(x)e^{i(k_y y + k_z z)}.$$

## 6.4 The Zeeman splitting of the Landau level

Here we consider the effect of the spin magnetic moment on the Landau level.

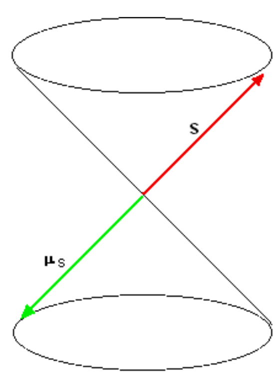



**Fig.21** Spin angular momentum ***S*** and spin magnetic moment $\boldsymbol{\mu}_s$ for free electron. $\mathbf{S} = \hbar\boldsymbol{\sigma}/2$. $\boldsymbol{\mu}_s = -(2\mu_B\mathbf{S}/\hbar)$. $\mu_B = e\hbar/2m_0c$ (Bohr magnetron).

The spin magnetic moment $\boldsymbol{\mu}_s$ is given by $\boldsymbol{\mu}_s = -g\mu_B(\mathbf{S}/\hbar) = -(g\mu_B/2)\boldsymbol{\sigma}$, where $\mu_B = e\hbar/(2m_0c)$ (Bohr magneton). The factor *g* is called the Landé-*g* factor and is equal to *g* =2.0023 for free electrons. In the presence of magnetic field ***B*** along the *z* axis, the Zeeman energy is given by

$$-\boldsymbol{\mu}_s \cdot \mathbf{B} = \frac{g\mu_B}{2} B\sigma = \hbar\omega_c \frac{m_c}{m_0}\left(\frac{g\sigma}{2}\right) = \frac{1}{2}\hbar\omega_c \nu_s \sigma\,, \qquad (72)$$

where $\nu_s = gm_c / m_0$ and $\sigma = \pm 1$. Thus we have the splitting of the Landau level in the presence of magnetic field as

$$E(n,\sigma) = \hbar\omega_c\left(n + \frac{1}{2} + \frac{1}{2}\nu_s\sigma\right). \qquad (73)$$

where $\nu_s$ is much smaller than 1 for Bi.

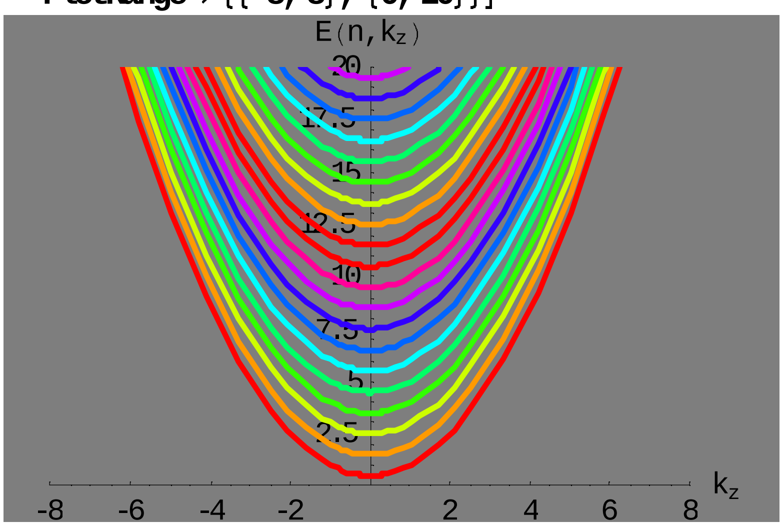
### 6.5 Numerical calculations using Mathematica 5.2

#### 6.5.1. ((Mathematica 5.2-1)) Energy dispersion of the Landau level

We consider the energy dispersion of the Landau level with the quantum number *n* as a function of $k_z$.

Here we assume that $\hbar \to 1$, $\omega_c \to 1$, and $m \to 1$ for numerical calculations. $n$ = 0,1, 2, …, 20.

```
G[n_] := ħ ωc (n+ 1/2) + ħ^2/(2 m) kz^2
 rule1={ħ→1,ωc→1,m→1}
 {ħ→1,ωc→1,m→1}
 G1=G[n]/.rule1
 1/2 + kz^2/2 + n
 Plot[Evaluate[Table[G1, {n, 0, 20}]], {kz, -10, 10},
  PlotStyle→ Table[Hue[0.1 i], {i, 0, 10}], Prolog→ AbsoluteThickness[2],
  Background→ GrayLevel[0.5], AxesLabel→ {"kz", "E(n,kz)"},
  PlotRange→ {{-8, 8}, {0, 20}}]
```




```
-Graphics-
```

**Fig.22** Energy dispersion of the Landau levels with *n* and $k_z$ for a 3D electron gas in the presence of a magnetic field along the *z* axis.

## 6.5.2. ((Mathematica 5.2-2)) Solution of Schrödinger equation

```
(*Landau level*)
πx := ℏ/ⅈ D[#, x] &
πy := (ℏ/ⅈ D[#, y] - e B x/c #) &
πy[ψ[x,y,z]]
```

$$-\frac{B e x \psi[x, y, z]}{c} - i \hbar \psi^{(0,1,0)}[x, y, z]$$

```
πy[πy[ψ[x,y,z]]]//Simplify
```

$$\frac{1}{c^2}\left(B^2 e^2 x^2 \psi[x, y, z] + c\hbar\left(2 i B e x \psi^{(0,1,0)}[x, y, z] - c\hbar\psi^{(0,2,0)}[x, y, z]\right)\right)$$

```
Nest[πy,ψ[x,y,z],2]//Simplify
```

$$\frac{1}{c^2}\left(B^2 e^2 x^2 \psi[x, y, z] + c\hbar\left(2 i B e x \psi^{(0,1,0)}[x, y, z] - c\hbar\psi^{(0,2,0)}[x, y, z]\right)\right)$$

```
πz := ℏ/ⅈ D[#, z] &
f =
  1/(2 m) (Nest[πx, ψ[x, y, z], 2] + Nest[πy, ψ[x, y, z], 2] +
     Nest[πz, ψ[x, y, z], 2]) == E1 ψ[x, y, z] // Simplify
```

$$\frac{1}{2c^2 m}\left(B^2 e^2 x^2 \psi[x, y, z] - c\hbar\left(c\hbar\psi^{(0,0,2)}[x, y, z] - 2 i B e x \psi^{(0,1,0)}[x, y, z] + c\hbar\left(\psi^{(0,2,0)}[x, y, z] + \psi^{(2,0,0)}[x, y, z]\right)\right)\right) == E1\,\psi[x, y, z]$$

```
(*We assume the form of wave function
     ψ[x,y,z]=(Exp[ⅈ ky y2 +ⅈ kz z] ϕ[x]

     *)
rule1={ψ→(Exp[ⅈ ky #2 +ⅈ kz #3] ϕ[#1]&)}
```

$$\left\{\psi \to \left(e^{i\,ky\#2 + i\,kz\#3}\,\phi[\#1]\ \&\right)\right\}$$

```
f1=f/.rule1//Simplify
```

$$\frac{1}{c\,m}\left(e^{i(ky\,y + kz\,z)}\left(\left(-B^2 e^2 x^2 + 2 B c e\,ky\,x\hbar + c^2\left(2 E1 m - \left(ky^2 + kz^2\right)\hbar^2\right)\right)\phi[x] + c^2\hbar^2\phi''[x]\right)\right) == 0$$

```
eq1 = ((-B^2 e^2 x^2 + 2 B c e ky x ℏ + c^2 (2 E1 m - (ky^2 + kz^2) ℏ^2)) ϕ[x] + c^2 ℏ^2 ϕ''[x]) == 0
```

$$\left(-B^2 e^2 x^2 + 2 B c e\,ky\,x\hbar + c^2\left(2 E1 m - \left(ky^2 + kz^2\right)\hbar^2\right)\right)\phi[x] + c^2\hbar^2\phi''[x] == 0$$

```
eq2 = Solve[eq1, ϕ''[x]] // Simplify // Flatten
```

$$\left\{\phi''[x] \to \frac{\left(B^2 e^2 x^2 - 2 B c e\,ky\,x\hbar + c^2\left(-2 E1 m + \left(ky^2 + kz^2\right)\hbar^2\right)\right)\phi[x]}{c^2\hbar^2}\right\}$$

```
eq3 = ϕ''[x] - (ϕ''[x] /. eq2) == 0
```

$$-\frac{(B^2 e^2 x^2 - 2 B c e\, ky\, x \hbar + c^2(-2 E1 m + (ky^2 + kz^2)\hbar^2))\phi[x]}{c^2\hbar^2} + \phi''[x] == 0$$

**vchange**[**Eq_**, **ψ_**, **x_**, **z_**, **f_**] :=

**Eq** /. {**D**[**ψ**[**x**], {**x**, **n_**}] :→ **Nest**[$\left(\frac{1}{D[f, z]} D[\#, z]\ \&\right)$, **ψ**[**z**], **n**],

**ψ**[**x**] :→ **ψ**[**z**], **x** :→ **f**}

(* **change of variable**

$x = \xi/\beta$, $\beta = \sqrt{\frac{m\,\omega c}{\hbar}} = \sqrt{\frac{e\,B}{\hbar\,c}}$, $\omega c = \frac{e\,B}{m\,c}$

**ξ is dimensionless**

*)

**seq1** = **vchange**[**eq3**, **ϕ**, **x**, **ξ**, $\frac{\xi}{\beta}$] // **FullSimplify**

$$\beta^2 \phi''[\xi] == \frac{1}{c^2\beta^2\hbar^2}\left((B^2 e^2 \xi^2 + c\beta(-2 B e\, ky\, \xi\hbar + c\beta(-2 E1 m + (ky^2 + kz^2)\hbar^2)))\phi[\xi]\right)$$

**rule2** = $\left\{\beta \to \sqrt{\frac{e\,B}{\hbar\,c}}\right\}$

$$\left\{\beta \to \sqrt{\frac{B e}{c \hbar}}\right\}$$

**seq2=seq1/.rule2//Simplify**

$$\frac{1}{c\hbar}\left(\left(-B e \xi^2 \hbar + c\left(2 E1 m - \left(ky^2 + kz^2 - 2\, ky\, \xi\sqrt{\frac{B e}{c\hbar}}\right)\hbar^2\right)\right)\phi[\xi] + B e \hbar \phi''[\xi]\right) == 0$$

**seq3** = **Solve**[**seq2**, **ϕ''**[**ξ**]] // **Simplify** // **Flatten**

$$\left\{\phi''[\xi] \to \frac{\left(B e \xi^2 \hbar + c\left(-2 E1 m + \left(ky^2 + kz^2 - 2\, ky\, \xi\sqrt{\frac{Be}{c\hbar}}\right)\hbar^2\right)\right)\phi[\xi]}{B e \hbar}\right\}$$

**seq4** = **ϕ''**[**ξ**] - (**ϕ''**[**ξ**] /. **seq3**) == **0** // **FullSimplify**

$$\phi''[\xi] == \frac{\left(B e \xi^2 \hbar + c\left(-2 E1 m + \left(ky^2 + kz^2 - 2\, ky\, \xi\sqrt{\frac{Be}{c\hbar}}\right)\hbar^2\right)\right)\phi[\xi]}{B e \hbar}$$

(*

$\xi 0 = \beta\ \frac{c\,\hbar\ ky}{e\,B} = \sqrt{\frac{e\,B}{\hbar\,c}}\ \frac{c\,\hbar\ ky}{e\,B} = \sqrt{\frac{c\,\hbar}{e\,B}}\ ky$

*)

**rule3** = $\left\{ky \to \sqrt{\frac{e\,B}{c\hbar}}\ \xi 0\right\}$

$$\left\{ky \to \xi 0 \sqrt{\frac{Be}{c\hbar}}\right\}$$

```
seq5=seq4/.rule3//Simplify
```

$$\phi''[\xi] == \frac{(Be(\xi-\xi 0)^2\hbar + c(-2\,E1\,m + kz^2\hbar^2))\,\phi[\xi]}{Be\hbar}$$

(*The energy E1

$$E1 = \hbar\ \omega C\left(n+\frac{1}{2}\right)+\frac{\hbar^2\ kz^2}{2\ m}$$

$$\hbar\ \omega C\ =\ \frac{e\ B\ \hbar}{m\ c}$$

*)

$$rule4 = \left\{E1 \to \frac{e\,B\hbar}{m\,c}\left(n+\frac{1}{2}\right)+\frac{\hbar^2 kz^2}{2\,m}\right\}$$

$$\left\{E1 \to \frac{Be\left(\frac{1}{2}+n\right)\hbar}{c\,m} + \frac{kz^2\hbar^2}{2\,m}\right\}$$

```
seq6=seq5/.rule4//Simplify
```

$$\phi''[\xi] == (-1-2n+\xi^2-2\xi\xi 0+\xi 0^2)\,\phi[\xi]$$

```
DSolve[seq6,φ[ξ],ξ]
```

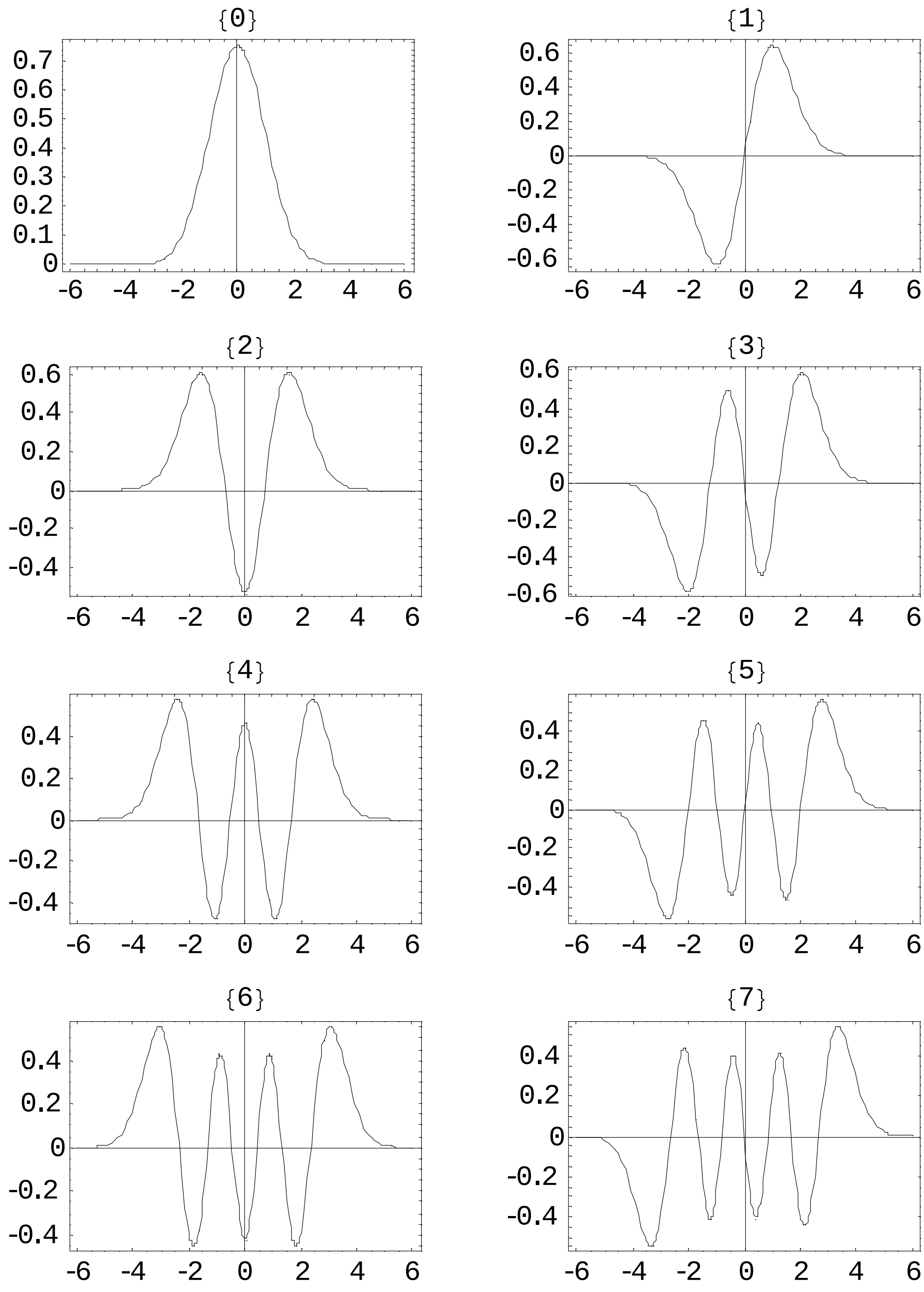
$$\left\{\left\{\phi[\xi] \to e^{-\frac{\xi^2}{2}+\xi\xi 0}\,C[1]\ \mathrm{HermiteH}[n,\ \xi-\xi 0] + e^{-\frac{\xi^2}{2}+\xi\xi 0}\,C[2]\ \mathrm{Hypergeometric1F1}\left[-\frac{n}{2},\ \frac{1}{2},\ (\xi-\xi 0)^2\right]\right\}\right\}$$

**6.5.3. ((Mathematica 5.2-3)) Plot of the Landau wave function as a function of $\xi$, where $\xi_0 = 0$.**

```
(*Simple Harmonics wave function*)
(*plot of φn[ξ]*)
conjugateRule = {Complex[re_, im_] :→ Complex[re, -im]};
Unprotect[SuperStar]; SuperStar /: exp_* := exp /. conjugateRule;
Protect[SuperStar]
{SuperStar}
```

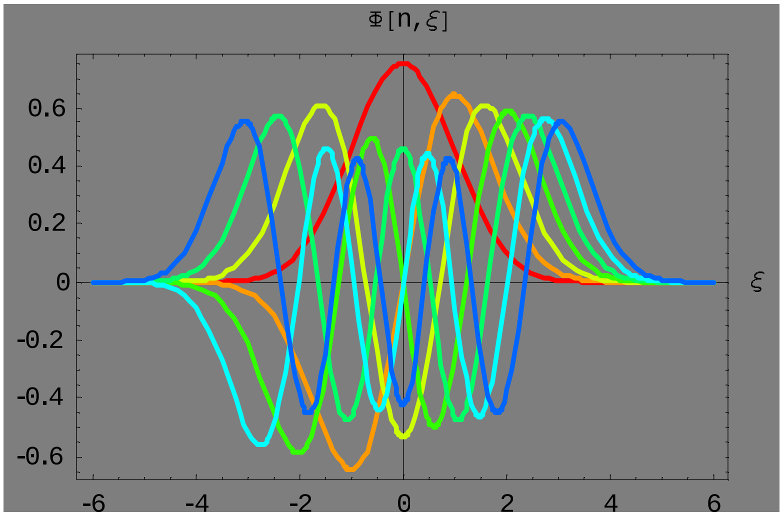
$$\psi[n\_,\ \xi\_] := 2^{-n/2}\ \pi^{-1/4}\ (n!)^{-1/2}\ \mathrm{Exp}\left[-\frac{\xi^2}{2}\right]\ \mathrm{HermiteH}[n,\ \xi]$$

```
pt1[n_]:=Plot[Evaluate[ψ[n,ξ]],{ξ,-6,6},PlotLabel→{n},PlotPoints→100,PlotRange→All,DisplayFunction→Identity,Frame→True]

pt2=Evaluate[Table[pt1[n],{n,0,8}]];Show[GraphicsArray[Partition[pt2,2]]]
```




-GraphicsArray-

```
Plot[Evaluate[Table[ ψ[n,ξ],{n,0,6}]],{ξ,-
6,6},Prolog→AbsoluteThickness[2],PlotStyle→Table[Hue[0.1
i],{i,0,8}],AxesLabel→{"ξ","
Φ[n,ξ]"},Frame→True,Background→GrayLevel[0.5]]
```




-Graphics-

**Fig.23** Plot of the wave function $\phi_n(\xi)$ with $\xi_0 = 0$ as a function of $\xi$. $n$ = 0, 1, …,and 6.

## 7. General form of the oscillatory magnetization (Lifshitz-Kosevich)

The expression of the oscillatory magnetization is derived by Lifshitz and Kosevich[11]as

$$M = -\frac{\sqrt{2}T(e\hbar/c)^{3/2}}{\pi^{3/2}B^{1/2}}\sum_e S_e\left|\frac{\partial^2 S}{\partial p_z^2}\right|_e^{-1/2}\exp\left(-\frac{2\pi^2 Tcm_c}{e\hbar B}\right)\sin\left(\frac{cS_e}{e\hbar B}\pm\frac{\pi}{4}\right)\cos\left(\frac{\pi m_c}{m_0}\right), \quad (74)$$

where the sum over $e$ extends all extremal cross-sectional are of the Fermi surface, the phase $+\pi/4$ if $\partial S/\partial p_z>0$ (minimum) and $-\pi/4$ if $\partial S/\partial p_z<0$ (maximum), $m_0$ is a mass of free electron, and $m_c = (1/2\pi)\partial S/\partial\varepsilon$. The term $\cos(\pi m_c/m_0)$ arises from the Zeeman splitting of spins. The magnetization oscillations are periodic in 1/$B$. The period is

$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e\hbar}{cS_e}, \quad (75)$$

The influence of electron scattering is not taken into account in the derivation given above. Its effect is easily estimated. A proper account of the influence of collisions gives rise to an additional factor. If the mean time between collisions is $\tau$, the corresponding uncertainty in electron energies $\hbar/\tau$ is equivalent to a temperature, so-called Dingle temperature

$$\exp\left(-\frac{2\pi^2 cm_c}{e\tau H}\right) = \exp\left(-\frac{2\pi^2 k_B T_d cm_c}{e\hbar H}\right), \quad (76)$$

where $T_d$ is the Dingle temperature and is defined by

$$T_d = \frac{\hbar}{k_B\tau}.$$

## 8. Simple model to understand the dHvA effect[13,16]

Consider the figure showing Landau levels associated with successive values of $n$ = 0, 1, 2, …, $s$. The upper green line represents the Fermi level $\varepsilon_F$. The levels below $\varepsilon_F$ are filled, those above are empty. Since $\varepsilon_F$ is much larger than the level-separation $\hbar\omega_c$, the number $n = s$ of occupied levels is very large. Let us assume that the magnetic field is increased slightly. The level separation will increase, and one of the lower levels will eventually cross the Fermi level. The resulting distribution of levels is similar to the original one except that the number of filled levels below $\varepsilon_F$ is now $n = s$-1, instead of $n = s$. Since $n$ is large, this difference is essentially negligible, so that one expects the new state to be equivalent to the original one. This implies a periodic dependence of the magnetization.

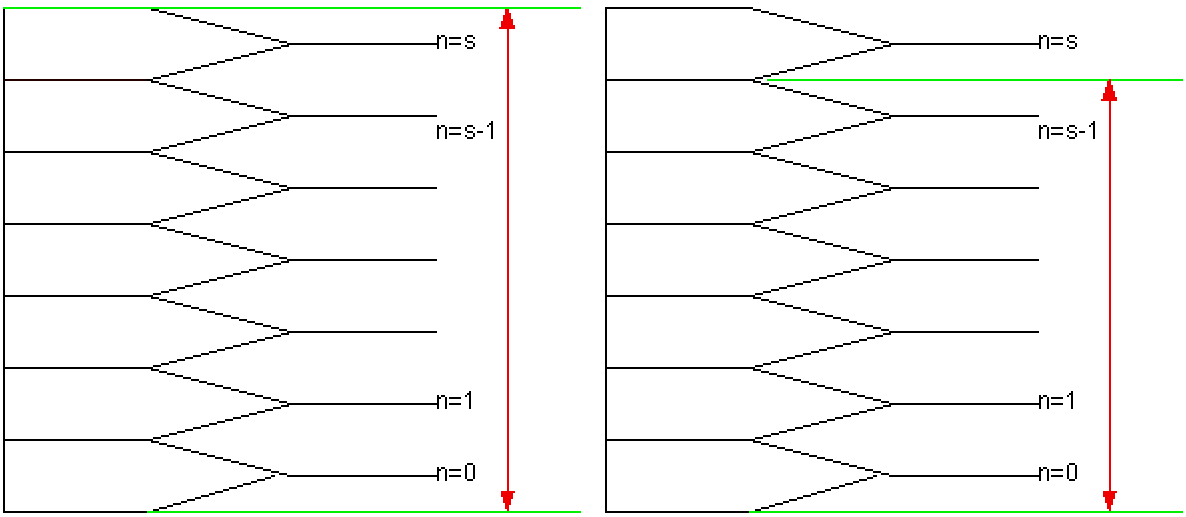
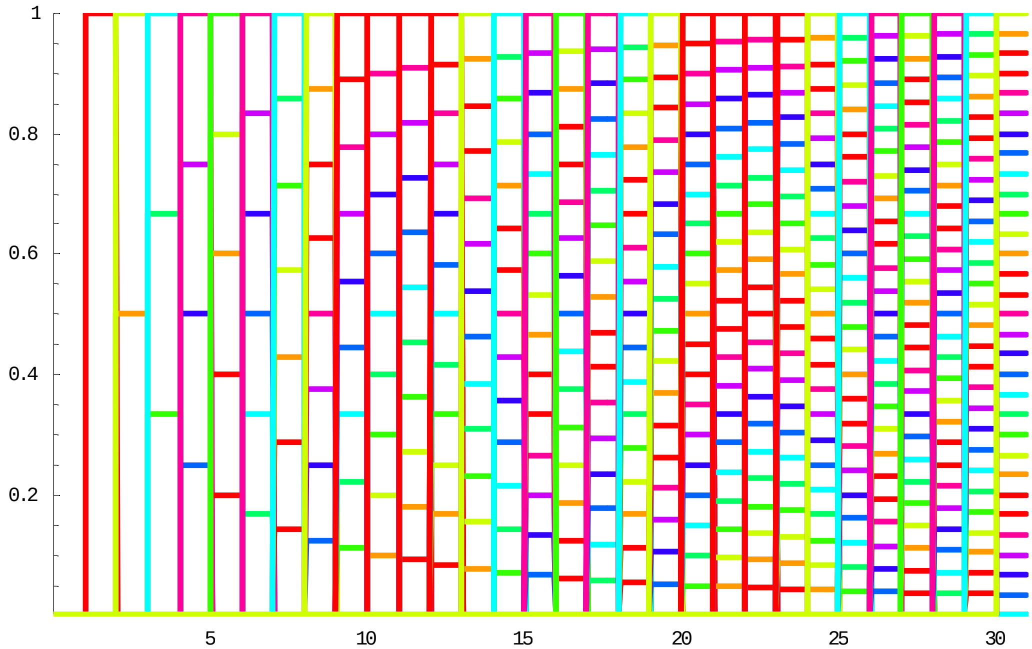



**Fig.24** Schematic energy diagram of a 2D free electron gas in the absence and presence of $B$. At $B = 0$, the states below $\varepsilon_F$ are occupied. The energy levels are split into the Landau levels with (a) $n$ = 0, 1, 2,…, and $s$ for a specified field and (b) $n$ = 0, 1, 2,…, and $s$-1 for another specified field. The total energy of the electrons is the same as in the absence of a magnetic field.

**((Mathematica 5.2-4)) Schematic energy diagram as a function of 1/B**

This figure shows the schematic diagram of the location of each Landau levels as a function of $\varepsilon_F/\hbar\omega_c$. When $\varepsilon_F/\hbar\omega_c = s$ (integer), there are s Landau levels below the Fermi level $\varepsilon_F$.

```
Plot[Evaluate[Table[i/n (UnitStep[x - n] - UnitStep[x - n - 1]), {n, 1, 30},
   {i, 1, n}]], {x, 0, 31}, Prolog → AbsoluteThickness[3],
 PlotStyle → Table[Hue[0.1 j], {j, 0, 10}], PlotRange → {{0, 31}, {0, 1}}]
```




-Graphics-

**Fig.25** Schematic diagram for the separation of the Landau level as a function of $1/B$. The $x$ axis is $s = N/(\rho B)$. The $y$ axis is equal to the energy normalized by the Fermi energy $\varepsilon_F$. The number of the Landau levels below $\varepsilon_F$ is equal to $s$ at $x = s$.

## 9. Derivation of the oscillatory behavior in a 2D model.

The energy level of each Landau level is given by $\hbar\omega_c(n+1/2)$, where $n$ = 0, 1, 2, ….. Each on of the Landau level is degenerate and contains $\rho B$ states. We now consider several cases.

(A) The $n$ = 0, 1, 2, …, $s$-1 states are occupied. $n = s$ state is empty.

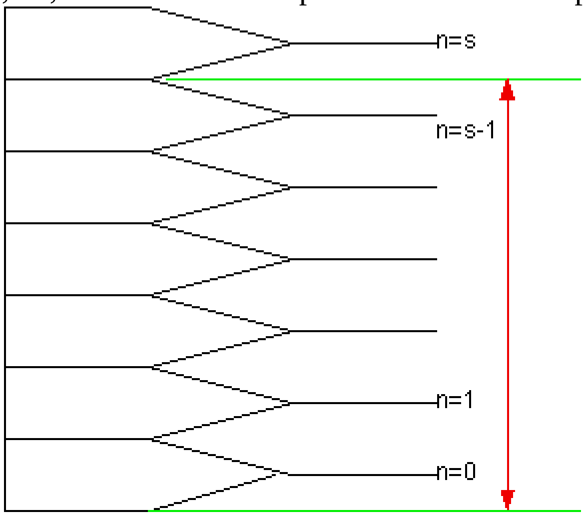



**Fig.26**

$$\varepsilon_F = \hbar\omega_c s\,.$$

$$N = \rho B s \,.$$

The total energy is constant,

$$U = U_0 = \sum_{n=0}^{s-1} \rho B (n + \frac{1}{2}) \hbar \omega_c = \hbar \omega_c \rho B [\frac{1}{2} s(s-1) + \frac{1}{2} s] = \hbar \omega_c \rho B \frac{1}{2} s^2 = \frac{1}{2} \varepsilon_F N \,. \qquad (77)$$

(B) The case where the $n = s$ state is not filled.

We now consider the case when $\hbar \omega_c$ decreases. This corresponds to the decrease of *B*.

(i) $\varepsilon < \hbar \omega_c / 2$, where $\varepsilon$ is the energy difference defined by the figure below.

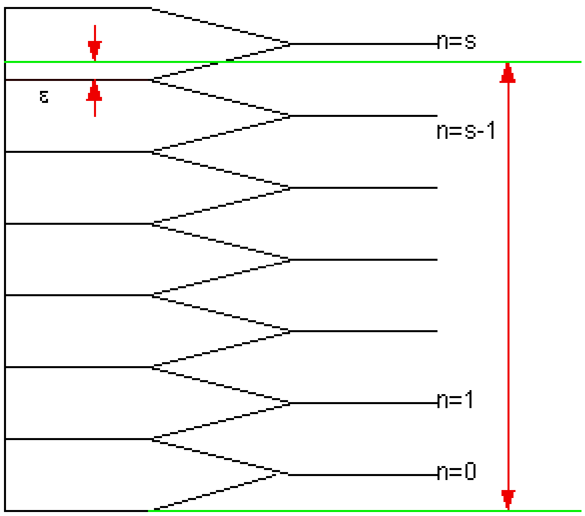



**Fig.27**

(ii) $\hbar \omega_c / 2 < \varepsilon < \hbar \omega_c$

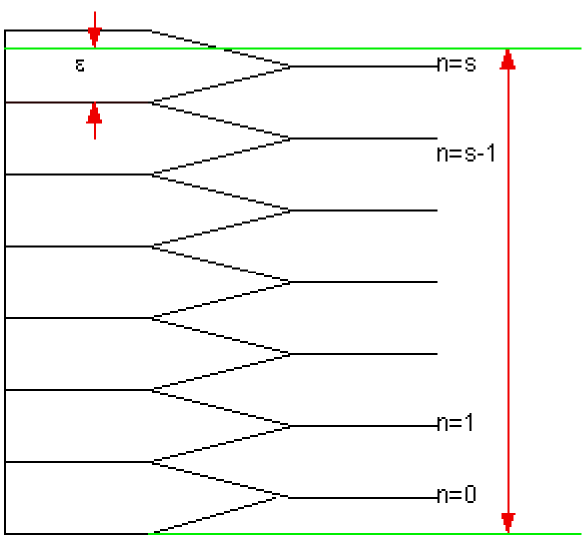



**Fig.28**

$$\varepsilon_F = s \hbar \omega_c + \varepsilon \,,$$

with $0 < \varepsilon < \hbar\omega_c$.

The $n$ = 0, 1, 2, …, ($s$-1) levels are occupied and the $n = s$ level is not filled.
The total number of electrons is $N$. The energy due to the partially occupied $n = s$ state is $(N - \rho Bs)\hbar\omega_c(s + \frac{1}{2})$. Then the total energy is

$$
\begin{aligned}
U - U_0 &= \sum_{n=0}^{s-1} \rho B(n + \frac{1}{2})\hbar\omega_c - \frac{1}{2}\varepsilon_F N + (N - \rho Bs)\hbar\omega_c(s + \frac{1}{2}) \\
&= \hbar\omega_c \rho B \frac{1}{2} s^2 - \frac{1}{2}\varepsilon_F N + (N - \rho Bs)\hbar\omega_c(s + \frac{1}{2}), \qquad (78)
\end{aligned}
$$

where

$$\rho Bs < N < \rho B(s+1), \qquad \text{and} \qquad s\hbar\omega_c < \varepsilon_F = (s+1)\hbar\omega_c.$$

Here we introduce $\lambda$ as

$$\lambda = N - \rho Bs.$$

The parameter $\lambda$ satisfies the inequality

$$0 < \lambda < \rho B,$$

for $\frac{\rho s}{N} < \frac{1}{B} < \frac{\rho(s+1)}{N}$. The parameter $\lambda$ denotes the number of electrons partially occupied in the $n = s$ state

The parameter $\mu = \rho Bs$ is the total number of electrons occupied in the $n$ = 0, 1, 2,…, $s$-1 states for $\frac{\rho s}{N} < \frac{1}{B} < \frac{\rho(s+1)}{N}$.

(iii) The $n$ = 0, 1, 2, …, $s$ states are occupied. $n = s$+1 state is empty.

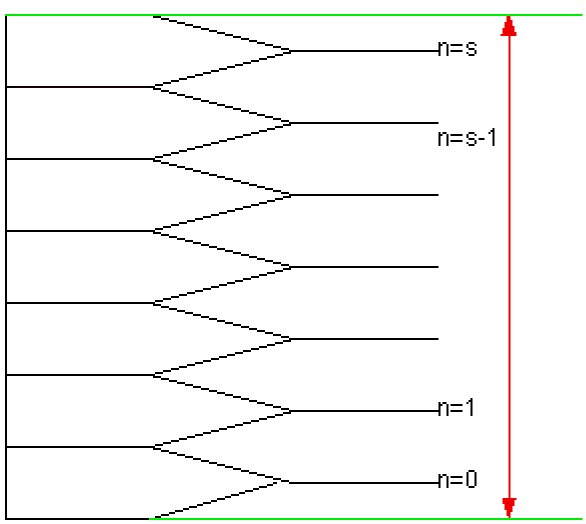



**Fig.29**

In this case we have

$$\varepsilon_F = \hbar\omega_c(s+1).$$

$N = \rho B(s+1)$.

$$U = U_0 = \sum_{n=0}^{s} \rho B(n+\frac{1}{2})\hbar\omega_c = \hbar\omega_c \rho B[\frac{1}{2}s(s+1) + \frac{1}{2}(s+1)]$$

$$= \hbar\omega_c \rho B \frac{1}{2}(s+1)^2 = \frac{1}{2}\varepsilon_F N$$

## 10. Total energy vs *B*

We now discuss the total energy as a function of *B*.

The total energy has a local minimum at $B = \dfrac{N(s+\frac{1}{2})}{\rho s(s+1)}$.

((Proof))
Since

$$\hbar\omega_c = \frac{\hbar e B}{m_c c} = 2(\frac{e\hbar}{2m_c c})B = 2\mu_B B,$$

the total energy is expressed by

$$U - U_0 = \hbar\omega_c \rho B \frac{1}{2}s^2 - \frac{1}{2}\varepsilon_F N + (N - \rho B s)\hbar\omega_c (s+\frac{1}{2})$$

$$= \mu_B \rho B^2 s^2 - \frac{1}{2}\varepsilon_F N + \mu_B B N(2s+1) - \mu_B \rho B^2 s(2s+1)$$

$$= -\frac{1}{2}\varepsilon_F N + \mu_B B N(2s+1) - \mu_B \rho B^2 s(s+1) = f(B).$$

$$f'(B) = \mu_B N(2s+1) - 2\mu_B \rho B s(s+1) = 0.$$

Then $f(B)$ has a local maximum at $B = \dfrac{N(s+\frac{1}{2})}{\rho s(s+1)}$,

or

$$\frac{1}{B} = \frac{\rho}{N}\frac{s(s+1)}{s+\frac{1}{2}}.$$

We also show that the total energy $f(B)$ becomes zero at

$$\frac{1}{B} = \frac{s\rho}{N} \text{ and } \frac{1}{B} = \frac{(s+1)\rho}{N}.$$

((Proof))
We note that $U$ - $U_0$=0 at

$$\varepsilon_F = \hbar\omega_c s, \quad \text{and} \quad N = \rho B s.$$

Then $\varepsilon_F = \hbar\omega_c s = \dfrac{e\hbar s}{m_c c}B = \dfrac{e\hbar}{m_c c}sB = 2\mu_B \dfrac{N}{\rho}$.

$$f(B) = -\mu_B \frac{N^2}{\rho} + \mu_B B N(2s+1) - \mu_B \rho B^2 s(s+1),$$

or

$$f(B) = -\frac{\mu_B}{\rho}[\rho^2 B^2 s(s+1) - N\rho B(2s+1) + N^2],$$

or

$$f(B) = -\mu_B \rho [B^2 s(s+1) - \frac{N}{\rho} B(2s+1) + \frac{N^2}{\rho^2}] = -\mu_B \rho (sB - \frac{N}{\rho})[(s+1)B - \frac{N}{\rho}].$$

The solution of $f(B) = 0$ is

$$\frac{1}{B} = \frac{s\rho}{N} \text{ and } \frac{1}{B} = \frac{(s+1)\rho}{N}.$$

## 11. Magnetization *M* vs *B*

The magnetization $M$ is given by

$$M = -\frac{\partial U}{\partial B} = -\frac{\partial B}{\partial x}\frac{\partial U}{\partial x} = x^2 \frac{\partial U}{\partial x} = x^2 \frac{N^2 \mu_B}{\rho}\frac{\partial F}{\partial x}, \qquad (79)$$

where

$$x = \frac{1}{B},$$

$$F = -s(s+1)\frac{\rho^2}{N^2}\frac{1}{x^2} + \frac{\rho}{N}(2s+1)\frac{1}{x} - 1,$$

$$\frac{\partial F}{\partial x} = 2s(s+1)\frac{\rho^2}{N^2}\frac{1}{x^3} - \frac{\rho}{N}(2s+1)\frac{1}{x^2},$$

$$M = x^2 \frac{N^2 \mu_B}{\rho}\frac{\partial F}{\partial x} = \frac{N^2 \mu_B}{\rho}[2s(s+1)\frac{\rho^2}{N^2}\frac{1}{x} - \frac{\rho}{N}(2s+1)].$$

$M = 0$ at

$$x = \frac{2s(s+1)}{2s+1}\frac{\rho}{N}.$$

**((Mathematica 5.2-5)) The Mathematica program is in the Appendix.**

In this numerical calculation we use $n = 10$, $\mu_B = 1$, and $\rho = 1.$ for simplicity.

```
(*de Haas van Alphen effect*)
U = -1/2 s (s + 1) μB ρ B^2 + N (s + 1/2) μB B - 1/2 N EF /. EF → μB N/ρ

B N (1/2 + s) μB - N^2 μB/(2 ρ) - 1/2 B^2 s (1 + s) μB ρ

eq1=D[U,B]

N (1/2 + s) μB - B s (1 + s) μB ρ

Solve[eq1==0,B]

{{B → N (1 + 2 s)/(2 (s + s^2) ρ)}}

U1[x_, s_] := U /. B → 1/x // Simplify

U1[x,s]
```

$$\frac{1}{2}\,\mu B\left(\frac{N+2Ns}{x}-\frac{N^2}{\rho}-\frac{s(1+s)\rho}{x^2}\right)$$

**U2 = U1[x, s] x^2 ρ / N^2 // PowerExpand // Simplify**

$$-\frac{\mu B\,(N^2 x^2 - N(1+2s)\,x\rho + s(1+s)\rho^2)}{2N^2}$$

**Solve[U2==0,x]//Simplify**

$$\left\{\left\{x\to\frac{s\rho}{N}\right\},\left\{x\to\frac{(1+s)\rho}{N}\right\}\right\}$$

**max1 = U1[x, s] /. {x → $\frac{s(1+s)\rho}{N\left(s+\frac{1}{2}\right)}$} // Simplify**

$$\frac{N^2\mu B}{8s\rho+8s^2\rho}$$

**rule1={N→10,ρ→1,μB→1}**

{N→10,ρ→1,μB→1}

**U2 = U1[x, s] (UnitStep[x − $\frac{s\rho}{N}$] − UnitStep[x − $\frac{(1+s)\rho}{N}$])**

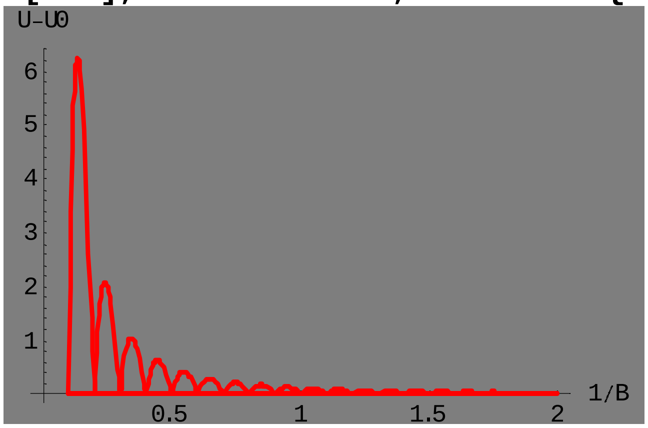
$$\frac{1}{2}\,\mu B\left(\frac{N+2Ns}{x}-\frac{N^2}{\rho}-\frac{s(1+s)\rho}{x^2}\right)\left(\text{UnitStep}\left[x-\frac{s\rho}{N}\right]-\text{UnitStep}\left[x-\frac{(1+s)\rho}{N}\right]\right)$$

**U4=U2/.{x→1/y}**

$$\frac{1}{2}\,\mu B\left((N+2Ns)\,y-\frac{N^2}{\rho}-s(1+s)\,y^2\rho\right)\left(\text{UnitStep}\left[\frac{1}{y}-\frac{s\rho}{N}\right]-\text{UnitStep}\left[\frac{1}{y}-\frac{(1+s)\rho}{N}\right]\right)$$

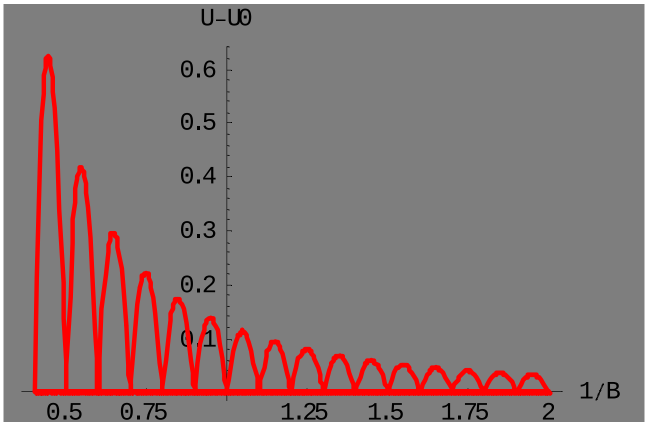
**(*Free energy as a function of x=1/B*)**

```
p11=Plot[Evaluate[Table[U2/.rule1,{s,0,20}]],{x,0.1,2},PlotStyle→Hue[0],Prolog→AbsoluteThickness[2],Background→GrayLevel[0.5],PlotPoints→50,AxesLabel→{"1/B","U-U0"}]
```




-Graphics-

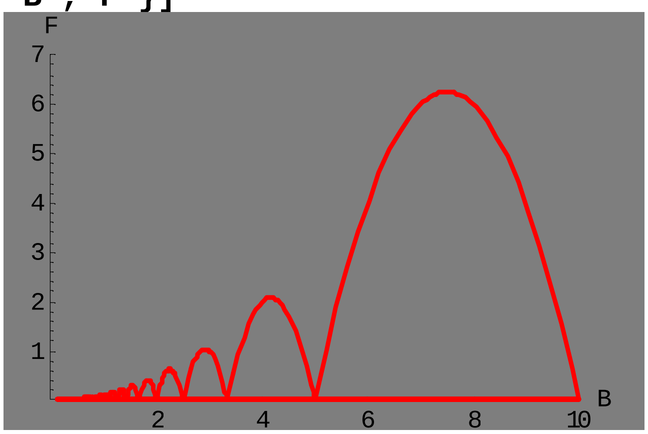
```
p110=Plot[Evaluate[Table[U2/.rule1,{s,0,20}]],{x,0.4,2},PlotStyle→Hue[0],Prolog→AbsoluteThickness[2],Background→GrayLevel[0.5],PlotPoints→100,AxesLabel→{"1/B","U-U0"}]
```




-Graphics-

**Fig.30** The plot of $U$-$U_0$ vs $1/B$ (the detail).

```
p111=Plot[Evaluate[Table[U4/.rule1,{s,0,20}]],{y,0.1,10},PlotStyle→Hue[0],Prolog→AbsoluteThickness[2],PlotPoints→50,PlotRange→{{0,10},{0,7}},Background→GrayLevel[0.5],AxesLabel→{"B","F"}]
```



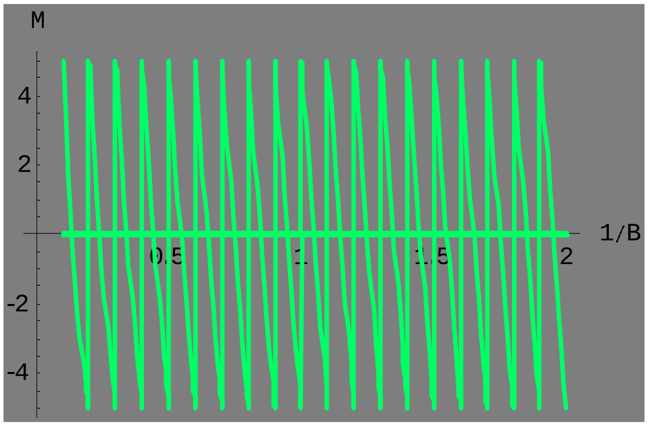

-Graphics-

**Fig.31** Plot of $U$-$U_0$ vs $B$.

```
M = x^2 D[U2, x] // Simplify
```

$$x^2\left(\frac{1}{2}\mu B\left(\frac{N+2Ns}{x}-\frac{N^2}{\rho}-\frac{s(1+s)\rho}{x^2}\right)\left(\text{DiracDelta}\left[x-\frac{s\rho}{N}\right]-\text{DiracDelta}\left[x-\frac{(1+s)\rho}{N}\right]\right)-\frac{1}{2x^3}\left(\mu B(N(x+2sx)-2s(1+s)\rho)\left(\text{UnitStep}\left[x-\frac{s\rho}{N}\right]-\text{UnitStep}\left[x-\frac{(1+s)\rho}{N}\right]\right)\right)\right)$$

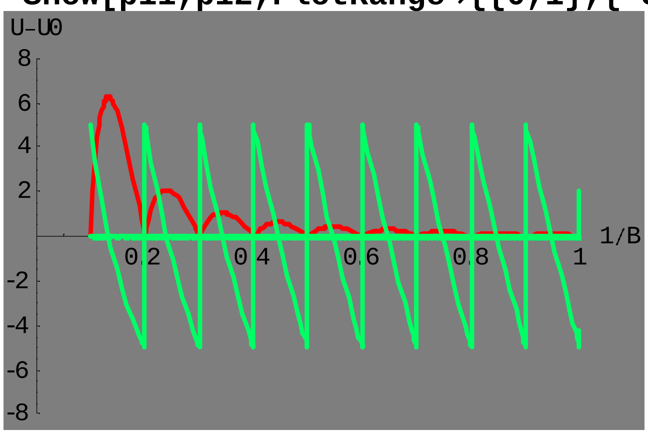
```
(*Magnetization as a function of 1/B*)

p12=Plot[Evaluate[Table[M/.rule1,{s,0,20}]],{x,0.1,2},PlotStyle→Hue[0.4],Prolog→AbsoluteThickness[2],Background→GrayLevel[0.5],PlotPoints→200,AxesLabel→{"1/B","M"}]
```




-Graphics-

**Fig.33** Plot of M vs 1/B

```
Show[p11,p12,PlotRange→{{0,1},{-8,8}}]
```




-Graphics-

**Fig.33** Plot of $U$-$U_0$ and $M$ as a function of 1/$B$.

```
(* The parameters λ=N-ρBs and μ=ρBs*)
NN1=N-ρ B s
```

N-B s ρ

```
NN2[x_,s_]=NN1/.B→1/x//Simplify
```

$N-\frac{s\,\rho}{x}$

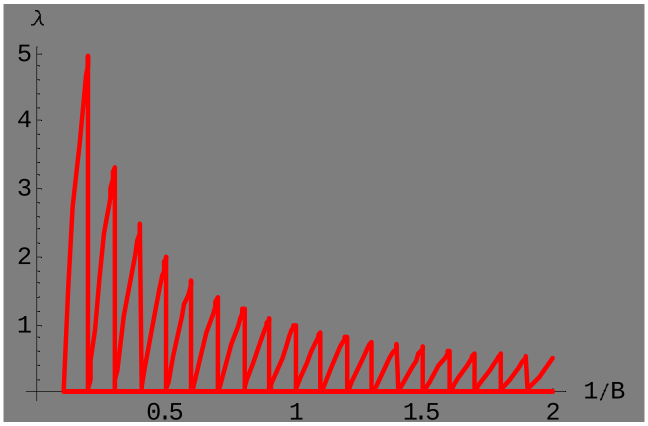
$$\mathbf{NN3}=\mathbf{NN2}[x,s]\left(\mathrm{UnitStep}\left[x-\frac{s\rho}{N}\right]-\mathrm{UnitStep}\left[x-\frac{(1+s)\rho}{N}\right]\right)$$

$$\left(N-\frac{s\rho}{x}\right)\left(\mathrm{UnitStep}\left[x-\frac{s\rho}{N}\right]-\mathrm{UnitStep}\left[x-\frac{(1+s)\rho}{N}\right]\right)$$

$$\mathbf{NN4}=\frac{s\rho}{x}\left(\mathrm{UnitStep}\left[x-\frac{s\rho}{N}\right]-\mathrm{UnitStep}\left[x-\frac{(1+s)\rho}{N}\right]\right)$$

$$\frac{s\rho\left(\mathrm{UnitStep}\left[x-\frac{s\rho}{N}\right]-\mathrm{UnitStep}\left[x-\frac{(1+s)\rho}{N}\right]\right)}{x}$$

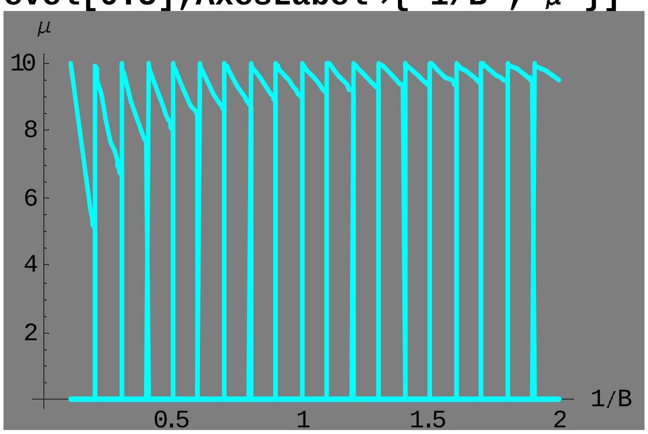
```
b11=Plot[Evaluate[Table[NN3/.rule1,{s,0,20}]],{x,0.1,2},Plot
Style→Hue[0],Prolog→AbsoluteThickness[2],Background→GrayLev
el[0.5],AxesLabel→{"1/B","λ"}]
```




-Graphics-

**Fig.34** Plot of $\lambda$ vs 1/*B* (red).

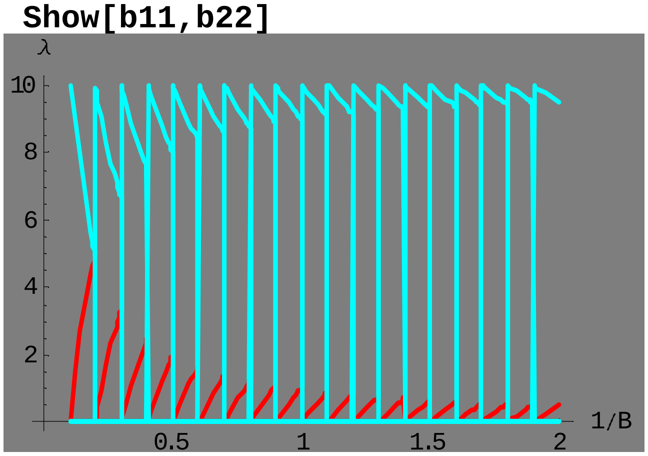
```
b22=Plot[Evaluate[Table[NN4/.rule1,{s,0,20}]],{x,0.1,2},Plot
Style→Hue[0.5],Prolog→AbsoluteThickness[2],Background→GrayL
evel[0.5],AxesLabel→{"1/B","μ"}]
```




-Graphics-

**Fig.35** Plot of $\mu$ vs 1/*B* (blue).

```
Show[b11,b22]
```




-Graphics-

**Fig.36** Plot of $\lambda$ vs 1/*B* (red) and $\mu$ vs 1/*B* (blue).

## 12. Conclusion

The physics on the dHvA effect of metals (in particular, bismuth) has been presented with the aid of Mathematica 5.2.

## Appendix

Mathematica 5.2 program (5) in Sec.10 is given, for convenience.

## REFERENCES


1. L. Landau, Z. Phys. **64**, 629 (1930).
2. L. Onsager, Phil. Mag. **43**, 1006 (1952).
3. D. Shoenberg, Proc. Roy. Soc. A **170**, 341 (1939).
4. M.H. Cohen, Phys. Rev. **121**, 387 (1962).
5. R.N. Brown, J.G. Mavroides, and B. Lax, Phys. Rev. **129**, 2055 (1963).
6. G.E. Smith, G.A. Baraff, and J.M. Rowell, Phys. Rev. B **135**, A1118 (1964).
7. R.N. Bhargrava, Phys. Rev. **156**, 785 (1967).
8. S. Takano and H. Kawamura, J. Phys. Soc. Jpn. **28**, 348 (1970).
9. M. Suzuki; Ph.D. Thesis at the University of Tokyo (1977).
10. M. Suzuki, H. Suematsu, and S. Tanuma, J. Phys. Soc. Jpn.**43**, 499 (1977).
11. I.M. Lifshitz and A.M. Kosevich, Sov. Phys. JETP **2**, 636 (1956).
12. A.B. Pippard, *Dynamics of conduction electrons*. (Gordon and Breach, New York, 1965).
13. A.A. Abrikosov, Solid State Physics Supplement 12, Introduction to the theory of normal metals, (Academic Press, New York, 1972).
14. D. Shoenberg, *Magnetic oscillations in metals*. (Cambridge University Press, London, 1984).
15. C. Kittel, *Introduction to Solid State Physics*, Sixth edition, (John Wiley and Sons Inc., New York, 1986).