Kapitel 2

Magnetism

2.1 Coupling of matter to a magnetic field: Diamagnetism and paramagnetism

An external magnetic field can couple to matter and electrons in two different ways (we consider the non-relativistic case):

(1) through the minimal coupling, expressed as

$$\vec{p} \to \vec{p} - \frac{e}{c}\vec{A}(\vec{r}), \tag{2.1}$$

where $\vec{p}$ is the momentum of the electron and $\vec{A}$ is the vector potential of the electromagnetic field,

(2) and through the spin of the electron, as

$$-\mu \cdot \vec{B} \approx \mu_B \vec{\sigma} \cdot \vec{B} \tag{2.2}$$

, with

$$\mu = -g\mu_B \vec{S}/\hbar = -g\mu_B\vec{\sigma}/2 \approx -\mu_B\vec{\sigma} \tag{2.3}$$

where $g \approx 2$ is the gyromagnetic factor for the free electron and $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$,

$$\mu_B = \frac{|e|\hbar}{2mc} > 0$$

is the Bohr magneton and $\vec{\sigma}$ are the Pauli matrices.

⋆ We will be using throughout the course *atomic units*. Since the distance between atoms in solids is of a few angstrom, the natural lengthscale is the Bohr radius a_0:

$$a_0 = \frac{\hbar^2}{me^2} = 0.5 \text{ angstrom} = 0.5 \times 10^{-8} \text{ cm}.$$

The energy scale is given in

$$E_0 = \frac{me^4}{\hbar^2} = \frac{e^2}{a_0} = 0.43 \times 10^{-10} \text{ erg} = 2 \text{ Ry} = 27.2 \text{ eV}.$$

The minimal coupling (2.1) is responsible for the *diamagnetism* in the system. The coupling to the spin, eq. (2.2), is the *Zeeman* coupling and is responsible for the *paramagnatism* in the system. From equations (2.1) and (2.2), we can write the Hamiltonian of an electron in a magnetic field $\vec{B}$ as

$$H = \frac{\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2}{2m} - \frac{e\hbar}{2mc}\vec{\sigma}\cdot\vec{B} + \underbrace{\frac{e\hbar^2}{4m^2c^2}\frac{1}{r}\frac{dV}{dr}\,\vec{l}\cdot\vec{\sigma}}_{\text{spin-orbit coupling}} + V(\vec{r}), \tag{2.4}$$

where $V(\vec{r})$ is the lattice potential. This Hamiltonian can be derived out of the Dirac equation.

Let us consider a static magnetic field applied along the z direction:

$$\begin{aligned} \vec{B} &= (0,0,B), \\ \vec{A} &= \frac{1}{2}(\vec{B}\times\vec{r}) = \frac{1}{2}(-By, Bx, 0) \quad \text{(symmetric gauge)} \end{aligned}$$

and

$$\begin{aligned} \left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 &= \vec{p}^{\,2} - \frac{e}{c}\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right) + \frac{e^2}{c^2}\vec{A}^2 \\ &= \vec{p}^{\,2} + \frac{eB}{2c}\left(p_x y + y p_x - p_y x - x p_y\right) + \frac{e^2B^2}{4c^2}(x^2+y^2). \end{aligned}$$

Then, the Hamiltonian (2.4) becomes

$$\boxed{H = \frac{\vec{p}^{\,2}}{2m} + \mu_B(l_z + \sigma_z)B + \frac{e^2B^2}{8mc^2}(x^2+y^2) + \frac{e\hbar^2}{4m^2c^2}\frac{1}{r}\frac{dV}{dr}\,\vec{l}\cdot\vec{\sigma} + V(\vec{r})}\,. \tag{2.5}$$

We note that

$$\begin{aligned} L_z &= xp_y - yp_x = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = \hbar l_z, \\ l_z &= \frac{1}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right), \\ S_z &= \frac{\hbar}{2}\sigma_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned}$$

Here, $\vec{L} = \hbar\vec{l}$ is the orbital angular momentum and $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$ is the spin. From eq. (2.5), we have that the external magnetic field couples linearly to the orbital angular momentum and the spin.

How does the system react to the application of external magnetic field? It is to be expected that the system will magnetize, therefore we should analyze the thermal expectation value of the magnetization:

$$\vec{M} = \langle\vec{\mu}\rangle = \mathrm{Tr}(\rho\vec{\mu}) = -\frac{\partial}{\partial\vec{B}}F_S,$$

where F_S is the free energy density of the system that can get magnetized. *Reminder*:

$$dF_S = -SdT - \vec{M}d\vec{B}.$$

The static (isothermal) magnetic susceptibility is then given by

$$\boxed{\chi_{\alpha\beta} = \frac{\partial M_\alpha}{\partial B_\beta} = -\frac{\partial}{\partial B_\beta}\frac{\partial}{\partial B_\alpha}F_S},$$

where $\chi_{\alpha\beta}$ is a tensor with components α and β. If we consider the equilibrium state, to which the system relaxes after application of a magnetic field, we can handle the system within equilibrium thermodynamics:

$$F_S = -k_BT\ln\sum_n e^{-\beta E_n}.$$

Here, E_n are the eigenvalues of the electron system in the presence of the external magnetic field. Then,

$$\vec{M} = -\frac{\partial F_S}{\partial \vec{B}} = \frac{-1}{\sum_n e^{-\beta E_n}}\sum_n \frac{\partial E_n}{\partial \vec{B}}e^{-\beta E_n},$$

which corresponds to

$$\boxed{\vec{M} = \langle\vec{\mu}\rangle = -\mu_B\langle\vec{l}+\vec{\sigma}\rangle = \frac{e\hbar}{2mc}\langle\vec{L}+2\vec{S}\rangle}.$$

The magnetization is obtained out of the thermal average of the magnetic moment $\vec{\mu}$. Since the electrons have negative charge ($e < 0$), the total magnetic moment has the opposite sign to orbital ($\vec{L}$) and spin ($\vec{S}$) moments.

If $\vec{B} = (0, 0, B)$, then

$$\begin{aligned}\chi_{zz} = \frac{\partial}{\partial B}M_z &= \frac{1}{\mathcal{Z}}\sum_n\left(\frac{1}{k_BT}\left(\frac{\partial E_n}{\partial B}\right)^2 - \frac{\partial^2 E_n}{\partial B^2}\right)e^{-\beta E_n}\\ &- \frac{1}{\mathcal{Z}^2 k_BT}\left(\sum_n\frac{\partial E_n}{\partial B}e^{-\beta E_n}\right)^2.\end{aligned}$$

with $\mathcal{Z} = \sum_n e^{-\beta E_n}$ being the partition function in the canonical ensemble.

In order to obtain the eigenvalues of the Hamiltonian (2.5), we apply perturbation theory up to the 2$^{\text{nd}}$ order in the magnetic field (see QM II course). The result reads as

$$\begin{aligned}E_n &= E_n^0 + \mu_B\langle n|l_z+\sigma_z|n\rangle B\\ &+ \frac{e^2B^2}{8mc^2}\langle n|(x^2+y^2)|n\rangle\\ &+ \mu_B^2\sum_{m\neq n}\frac{|\langle n|l_z+\sigma_z|m\rangle|^2B^2}{E_n^0 - E_m^0},\end{aligned}$$

where E_0 are the eigenvalues of the unperturbed Hamiltonian
In the limit $B \to 0$,

$$\begin{aligned} \frac{\partial E_n}{\partial B} &= \mu_B \langle n | l_z + \sigma_z | n \rangle, \\ \frac{\partial^2 E_n}{\partial B_n^2} &= \frac{e^2}{4mc^2} \langle n | y^2 + x^2 | n \rangle + 2\mu_B^2 \sum_{m \neq n} \frac{|\langle n | l_z + \sigma_z | m \rangle|^2}{E_n^0 - E_m^0}. \end{aligned} \tag{2.6}$$

In the absence of collective magnetism due to interaction among the electrons, we have for $B \to 0$ that

$$M_z = -\frac{1}{\mathcal{Z}} \sum_n \frac{\partial E_n}{\partial B} e^{-\beta E_n} = -\frac{1}{\mathcal{Z}} \sum_n e^{-\beta E_n^0} \mu_B \langle n | l_z + \sigma_z | n \rangle = \langle \mu_z \rangle = 0,$$

i. e., the magnetization disappears, since the magnetic moments thermally compensate. From eq. (2.6) we can divide the static susceptibility into three terms:

$$\chi_{zz} = \chi_{\mathrm{C}} + \chi_{\mathrm{vV}} + \chi_{\mathrm{dia}},$$

with

$$\chi_{\mathrm{C}} = \frac{\mu_B^2}{k_B T} \frac{\sum_n (\langle n | l_z + \sigma_z | n \rangle)^2 e^{-\beta E_n}}{\sum_n e^{-\beta E_n}} = \frac{\langle \mu_z^2 \rangle}{k_B T} > 0 \tag{2.7}$$

being the paramagnetic contribution,

$$\chi_{\mathrm{vV}} = -2 \frac{1}{\sum_n e^{-\beta E_n}} \sum_n \left\{ e^{-\beta E_n} \sum_{m \neq n} \mu_B \frac{|\langle n | l_z + \sigma_z | m \rangle|^2}{E_n^0 - E_m^0} \right\} \tag{2.8}$$

the van Vleck susceptibility and

$$\chi_{\mathrm{dia}} = -2 \frac{e^2}{8mc^2} \langle x^2 + y^2 \rangle = -\frac{e^2}{6mc^2} \langle r^2 \rangle < 0 \tag{2.9}$$

the diamagnetic contribution.

The paramagnetic contribution, eq. (2.7), is positive and has a $1/T$-temperature dependence:

$$\chi_{\mathrm{C}} = \frac{C}{T}, \quad \text{with} \quad \boxed{C = \frac{\mu_B^2}{k_B} \frac{1}{\mathcal{Z}} \sum_n \langle n | (l_z + \sigma_z) | n \rangle^2} \; e^{-\beta E_n}$$

being the Curie constant. Please note that even when the magnetization is zero, χ_{C} is different from zero and the system is in the paramagnetic state.

The paramagnetic contribution, eq. (2.8), is constant and positive since the eigenvalues of the excited states $|m\rangle$ are larger than the ground state energy: $E_m^0 > E_n^0$. This term will be significant when

$$k_B T \ll E_m^0 - E_n^0$$

i.e., at low temperature. For $k_B T \gg E_m^0 - E_n^0$, the van Vleck term has a $1/T$-behavior like the Curie term.

The diamagnetic contribution, eq. (2.9), is negative, which implies that the magnetization of the system for small fields has opposite sign to the magnetic field. This is a purely quantum effect. It comes from the term $\vec{p} \to \vec{p} - \frac{e}{c}\vec{A}$. Usually, the paramagnetic contribution is larger than the diamagnetic contribution, but if the total angular momentum disappears, there is no paramagnetic contribution and we are left with only the diamagnetic contribution (see below). This is called the Larmor diamagnetism.

In this section, we considered *one* electron under the influence of a magnetic field. We will generalize these results to a system of N non-interacting electrons.

2.2 Paramagnetism of localized magnetic moments

We consider a system of N atoms or ions with partially filled electron shells. The total magnetic moment per atom/ion is given by

$$\vec{J} = \vec{L} + \vec{S}.$$

In this case, we are dealing with *localized* magnetic moments, which correspond to the electrons in the partially filled shells and are localized on the atoms/ions, i.e. we are dealing with *insulators*. Let us consider the following two cases.

1) The electron shell has $J = 0$, which would be so in, for instance, shells with $S = 2$ and $L = 2$:

$$\vec{J} = \vec{L} + \vec{S},$$

$$|J| = |L - S|, |L - S| + 1, \ldots, L + S,$$

$$J = |L - S| = 0.$$

In this case, the linear term $\langle n|\vec{L} + \vec{S}|n\rangle$ disappears, and only the higher order terms (van Vleck paramagnetism and Larmor diamagnetism) contribute.

2) If the shell does not have $J = 0$, the linear term does not disappear and will dominate the magnetic behavior of the system. Please note that the ground state is $(2J + 1)$-fold degenerate in zero field. We can define the magnetic moment as

$$\vec{\mu} = -\tilde{g}\mu_B \frac{\vec{J}}{\hbar},$$

in the following we will set $\hbar$ to 1 and therefore J will be dimensionless.

$\boxed{\tilde{g}}$ is the Landé factor

$$\tilde{g} = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}.$$

In the following we will be using $g = \tilde{g}$. We consider now the simplest Hamiltonian where we neglect the diamagnetic contribution:

$$H = -\sum_i \vec{\mu}\vec{B} = \sum_i g\mu_B J_z B,$$

with $\vec{B} = (0,0,B)$, and calculate the susceptibility for the N atoms:

$$\mathcal{Z} \quad = \quad \mathrm{Tr}\ e^{-\beta H} = \mathrm{Tr}\ e^{-\beta\sum_i g\mu_B B J_z} = \prod_{i=1}^{N} \sum_{m_J=-J}^{+J} e^{-g\beta\mu_B B m_J}$$

We make use of

$$\sum_{k=0}^{n} ar^k = a\frac{1-r^{n+1}}{1-r} \tag{2.10}$$

then

$$\begin{aligned} \mathcal{Z} &= \prod_{i=1}^{N} \frac{e^{-g\mu_B BJ}(1-e^{g\mu_B B(2J+1)\beta})}{1-e^{g\mu_B B\beta}} \\ &= \prod_{i=1}^{N} \frac{e^{g\mu_B B(J+\frac{1}{2})\beta} - e^{-g\mu_B B(J+\frac{1}{2})\beta}}{e^{g\mu_B B\beta\frac{1}{2}} - e^{-g\mu_B B\beta\frac{1}{2}}}. \end{aligned}$$

Then, the free energy is

$$F = -k_B T \ln \mathcal{Z} = -Nk_B T \ln \frac{e^{g\mu_B B(J+\frac{1}{2})\beta} - e^{-g\mu_B B(J+\frac{1}{2})\beta}}{e^{g\mu_B B\beta\frac{1}{2}} - e^{-g\mu_B B\beta\frac{1}{2}}}$$

and the magnetization

$$\begin{aligned} M &= -\frac{\partial}{\partial B}F, \\ M &= Ng\mu_B\left((J+\frac{1}{2})\coth\left(\beta g\mu_B B(J+\frac{1}{2})\right) - \frac{1}{2}coth\left(g\mu_B\beta\frac{1}{2}\right)\right) \\ &= Ng\mu_B J\mathcal{B}_J(gJ\mu_B B\beta), \end{aligned}$$

where

$$\mathcal{B}_J(x) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J}\coth\left(\frac{x}{2J}\right)$$

is the Brillouin function. This function is shown in Fig. 2.1. For $x \ll 1$ it is linear and for $x \gg 1$ $\mathcal{B}_J(x) \to 1$ and $M \to Ng\mu_B J$, the saturation magnetization.

For small magnetic fields,

$$\coth(x) \approx \frac{1}{x} + \frac{x}{3} + \ldots$$

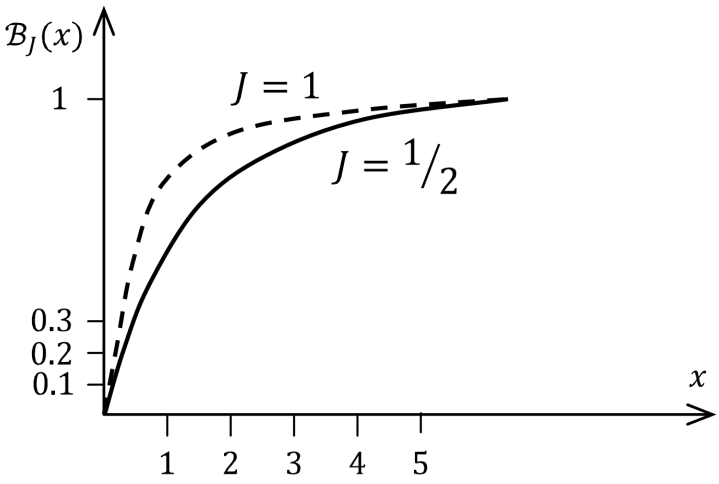


Abbildung 2.1: The Brillouin function.

so that

$$\mathcal{B}_J(x) \approx \left(1 + \frac{1}{J}\right)\frac{x}{3},$$

$$M \approx N\frac{J+1}{J} g\mu_B J \frac{g\mu_B J B\beta}{3} = N\frac{(g\mu_B)^2 J(J+1)}{3k_B T} B$$

and

$$\chi = \left.\frac{\partial M}{\partial B}\right|_{B\to 0} = N\frac{(g\mu_B)^2 J(J+1)}{3k_B T}$$

$$\Rightarrow \quad \chi = \frac{C}{T} \quad \text{with} \quad C = N\frac{J(J+1)}{3k_B}(g\mu_B)^2.$$

For spin-$\frac{1}{2}$ systems,

$$J = S = \frac{1}{2}, \qquad g = 2, \qquad C = N\frac{\mu_B^2}{k_B}.$$

Then,

$$\mathcal{B}_{1/2}(x) = \tanh(x)$$

and

$$\boxed{M = N\mu_B \tanh\left(\frac{\mu_B B}{k_B T}\right)}.$$

2.3 Pauli paramagnetism of conduction electrons

In the previous section, we considered localized moments. In the present section, we shall deal with conduction electrons in a metal. The electrons have a spin and the application of a magnetic field induces their magnetization. Therefore, we also expect a paramagnetic contribution from the conduction electrons.

Let us consider a minimal model where the spin of the conduction electrons is coupled to an external magnetic field:

$$H = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \mu_B B \sum_{\vec{k}} (c^\dagger_{\vec{k}\uparrow} c_{\vec{k}\uparrow} - c^\dagger_{\vec{k}\downarrow} c_{\vec{k}\downarrow}). \tag{2.11}$$

The z-component of all electron spins is

$$S_z = \frac{1}{2} \sum_{\vec{R}} (c^\dagger_{\vec{R}\uparrow} c_{\vec{R}\uparrow} - c^\dagger_{\vec{R}\downarrow} c_{\vec{R}\downarrow}) = \frac{1}{2} \sum_{\vec{k}} (c^\dagger_{\vec{k}\uparrow} c_{\vec{k}\uparrow} - c^\dagger_{\vec{k}\downarrow} c_{\vec{k}\downarrow})$$

and

$$\mu_z = -g\mu_B S_z = -\mu_B \sum_{\vec{k}} (c^\dagger_{\vec{k}\uparrow} c_{\vec{k}\uparrow} - c^\dagger_{\vec{k}\downarrow} c_{\vec{k}\downarrow}).$$

We calculate now the magnetization due to the application of an external magnetic field $\vec{B} = (0, 0, B)$:

$$M = \langle \mu_z \rangle = -\mu_B \sum_{\vec{k}} (\langle c^\dagger_{\vec{k}\uparrow} c_{\vec{k}\uparrow} \rangle - \langle c^\dagger_{\vec{k}\downarrow} c_{\vec{k}\downarrow} \rangle). \tag{2.12}$$

The Hamiltonian (2.11) can be rewritten as

$$H = \sum_{\vec{k}} (\varepsilon_{\vec{k}} + \mu_B B) c^\dagger_{\vec{k}\uparrow} c_{\vec{k}\uparrow} + \sum_{\vec{k}} (\varepsilon_{\vec{k}} - \mu_B B) c^\dagger_{\vec{k}\downarrow} c_{\vec{k}\downarrow}$$

so that we have free electrons with slightly displaced one-particle energies: $\varepsilon \pm \mu_B B$ (see Fig. 2.2).
Therefore, the expectation value in eq. (2.12) can be calculated through the Fermi function:

$$M = -\mu_B \int d\varepsilon \left[f(\varepsilon + \mu_B B) \rho_0(\varepsilon + \mu_B B) - f(\varepsilon - \mu_B B) \rho_0(\varepsilon - \mu_B B) \right],$$

where $\rho_0(\varepsilon)$ is the density of states of the free electrons. For small B, we perform a Taylor expansion:

$$M = -2\mu_B^2 B \int d\varepsilon \ \rho_0(\varepsilon) \frac{df}{d\varepsilon} = 2\mu_B^2 B \int d\varepsilon \ \rho_0(\varepsilon) \left(-\frac{df}{d\varepsilon} \right), \qquad -\frac{df}{d\varepsilon} = \delta(\varepsilon - \varepsilon_F).$$

Then,

$$\boxed{M = 2\mu_B^2 B \rho_0(\varepsilon_F)}$$

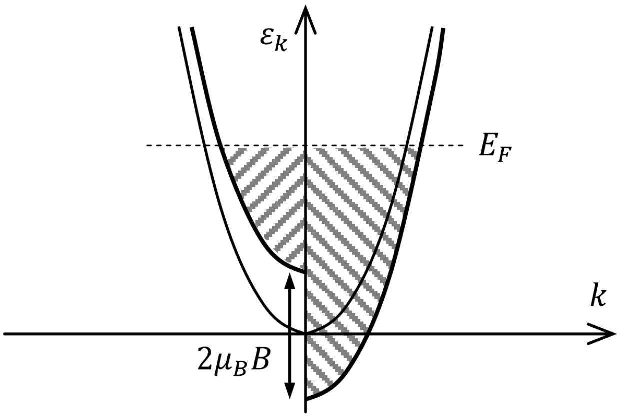


Abbildung 2.2: Energy spectrum of the conduction electrons in an external magnetic field.

and

$$\boxed{\chi_{\text{Pauli}} = 2\mu_B^2 \rho_0(\varepsilon_F)}$$

is the Pauli susceptibility (only valid for small B). Therefore, one expects in metals at low temperature a constant contribution to the susceptibility.

2.4 Landau diamagnetism

In the previous section, we dealt with the coupling of the spins of conduction electrons to an external magnetic field. The conduction electrons have also a well defined $\vec{p}$, and therefore we will also have a *diamagnetic* contribution due to the diamagnetic coupling to the magnetic field:

$$\vec{p} \to \vec{p} - \frac{e}{c}\vec{A}.$$

In order to analyze only this coupling, we consider spinless fermions in a magnetic field. In this case, the Hamilton operator is

$$\begin{aligned} H &= \sum_{i=1}^{N} \frac{\left(\vec{p}_i - \frac{e}{c}\vec{A}(\vec{r}_i)\right)^2}{2m} \\ &= \sum_i \frac{1}{2m}\left(\vec{p}_i - \frac{e}{c}\vec{p}_i\vec{A}_i(\vec{r}_i) - \frac{e}{c}\vec{A}_i(\vec{r}_i)\vec{p}_i + \frac{e^2}{c^2}\vec{A}^2(\vec{r}_i)\right). \end{aligned}$$

For the magnetic field given as $\vec{B} = (0,0,B)$ and the Landau gauge,

$$\vec{A} = (0, Bx, 0), \qquad \text{div}\vec{A} = 0 \quad \Rightarrow \quad \vec{p}\vec{A} = \vec{A}\vec{p},$$

the Hamiltonian reads

$$H = \sum_i \left(\frac{p_{ix}^2}{2m} + \frac{p_{iy}^2}{2m} + \frac{p_{iz}^2}{2m} - \frac{eB}{mc}p_{iy}x_i + \frac{e^2B^2}{2mc^2}x_i^2\right).$$

Since we are considering non-interacting electrons, we concentrate on the H for one electron:

$$\boxed{H_i = \frac{p_x^2}{2m} + \frac{m}{2}\omega_o^2\left(x - \frac{p_y}{m\omega_o}\right)^2 + \frac{p_z^2}{2m}},$$

where

$$\omega_o = \frac{eB}{mc}$$

is the *cyclotron frequency*, which corresponds to the classical frequency of particles in a magnetic field due to the Lorentz force in the xy plane. We consider the following one-particle wavefunction:

$$\Psi(\vec{r}) = C\varphi(x)e^{ik_y y}e^{ik_z z}.$$

Here, C is a normalization constant, and the y- and z-dependences are given in plane waves since the Hamiltonian does not depend explicitly on either y or z. Then,

$$\begin{aligned} H\Psi(\vec{r}) &= \left(\frac{p_x^2}{2m} + \frac{m}{2}\omega_0^2\left(x - \frac{\hbar k_y}{m\omega_0}\right)^2 + \frac{\hbar^2 k_z^2}{2m}\right) C\varphi(x)e^{ik_y y}e^{ik_z z} \\ &= EC\varphi(x)e^{ik_y y}e^{ik_z z}. \end{aligned}$$

We are left with a displaced harmonic oscillator for the x coordinate:

$$\varphi(x) = \varphi_n\left(\frac{x - x_0}{\lambda}\right),$$

where

$$\begin{aligned} x_0 &= \frac{\hbar k_y}{m\omega_0} = \frac{\hbar c k_y}{eB}, \\ \lambda &= \sqrt{\frac{\hbar}{m\omega_0}} = \sqrt{\frac{\hbar c}{eB}}. \end{aligned}$$

$\varphi(x)$ are the Hermite polynomials. The eigenvalues of H are

$$\boxed{E_{n,k_y,k_z} = \hbar\omega_0\left(n + \frac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m}},$$

with n being the Landau quantum number.

Instead of free electrons with dispersion

$$\varepsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m},$$

we now have free electrons with one-particle energies E_{n,k_y,k_z}, which are determined through three quantum numbers: the Landau quantum number n, k_y and k_z. The energy, however, has no explicit dependence on k_y. Therefore, we have degeneracy in the Landau level. This degeneracy is determined from the following condition for x_0:

$$x_0 = \frac{\hbar k_y}{m\omega_0} \leq L_x.$$

On the other hand, we have periodic boundary conditions in y:

$$k_y = \frac{2\pi}{L_y} l_y \quad \text{with} \quad l_y \in N.$$

Then,

$$\frac{2\pi\hbar}{m\omega_0 L_y} l_y \leq L_x \quad \Rightarrow \quad l_y \leq \frac{m\omega_0 L_x L_y}{2\pi\hbar},$$

which implies that the number of allowed l_y, defining the degeneracy of a Landau level, is

$$\frac{m\omega_0 L_y L_x}{2\pi\hbar} = \frac{|e|B}{c}\frac{L_x L_y}{2\pi\hbar}.$$

Let us calculate the contribution of the Landau diamagnetism to the susceptibility by considering the thermodynamic relations. We can work either in the canonical or in the grand canonical ensemble:

$$\begin{aligned}
\Phi &= -2k_B T \sum_\alpha \ln\left(1 + e^{-\beta(\varepsilon_\alpha - \mu)}\right) \\
&= -2k_B T \frac{L_z}{2\pi\hbar} \int dk_z \frac{|e|B}{c}\frac{L_x L_y}{2\pi\hbar} \sum_{n=0}^{\infty} \ln\left(1 + e^{-\beta(\varepsilon_\alpha - \mu)}\right) \\
&= -\frac{k_B T}{2\pi^2}\frac{V}{\hbar^2}\frac{|e|B}{c} \sum_{n=0}^{\infty} \int dk_z \ln\left[1 + e^{-\beta(\hbar\omega_0(n+\frac{1}{2}) + \frac{\hbar^2 k_z^2}{2m} - \mu)}\right],
\end{aligned}$$

which can be written as

$$\Phi = \frac{-|e|k_B T V}{2\pi^2\hbar^2}\frac{B}{c}\sum_{n=0}^{\infty} g(\mu - \hbar\omega_0(n+\frac{1}{2})),$$

where

$$g(\mu - x) = \int dk_z \ln\left(1 + e^{\beta(\mu - x - \frac{\hbar^2 k_z^2}{2m})}\right).$$

In order to perform the sum over the Landau quantum number, we can use the Euler-Maclaurin formula:

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

Then,

$$\begin{aligned}
\sum_{n=0}^{\infty} g(\mu - \hbar\omega_0(n+\frac{1}{2})) &= \int_0^\infty g(\mu - \hbar\omega_0 x)dx + \frac{1}{24}\frac{d}{dx}g(x)\Big|_{x=0} \\
&= \frac{1}{\hbar\omega_0}\int_{-\infty}^{\mu} dy\, g(y) - \frac{\hbar\omega_0}{24}\frac{d}{dy}g(y)\Big|_{y=\mu},
\end{aligned}$$

with $y = \mu - \hbar\omega_0 x$. The grand canonical potential then becomes

$$\Phi = \frac{k_B T m}{2\pi^2\hbar^3} V \left[\underbrace{\int_{-\infty}^{\mu} dy\, g(y)}_{B-\text{independent}} - \frac{(\hbar\omega_0)^2}{24} \frac{d}{dy} g(y)\bigg|_{\mu} \right].$$

It can be written as

$$\Phi = \Phi_0(T,\mu) - \frac{\hbar^2 e^2 B^2}{24 m^2 c^2} \frac{\partial^2}{\partial\mu^2} \Phi_0(T,\mu),$$

with

$$\Phi_0(T,\mu) = \frac{k_B T m}{2\pi^2\hbar^3} V \int_{-\infty}^{\mu} dy\, g(y) = \frac{k_B T m}{2\pi^2\hbar^3} V \int_{-\infty}^{\mu} dy \int dk_z \ln\left(1 + e^{\beta(y - \frac{\hbar^2 k_z^2}{2m})}\right).$$

Then,

$$M = -\frac{\partial\Phi}{\partial B} = \frac{e^2\hbar^2}{12 m^2 c^2}\, B\, \frac{\partial^2\Phi_0}{\partial\mu^2}$$

and

$$\chi = \frac{\partial M}{\partial B} = \frac{e^2\hbar^2}{12 m^2 c^2} \frac{\partial^2\Phi_0}{\partial\mu^2}.$$

Therefore, the Landau susceptibility is

$$\chi_{\text{Landau}} = \frac{1}{3}\, \mu_B^2\, \frac{\partial^2\Phi_0}{\partial\mu^2}.$$

For Φ_0, we directly take the grand canonical potential for free electrons without magnetic field:

$$\begin{aligned}
\Phi_0 &= -2k_B T \sum_{\vec{k}} \ln\left(1 + e^{-\beta(\varepsilon_{\vec{k}} - \mu)}\right), \\
\frac{\partial\Phi_0}{\partial\mu} &= -2\sum_{\vec{k}} \frac{e^{-\beta(\varepsilon_{\vec{k}}-\mu)}}{1 + e^{-\beta(\varepsilon_{\vec{k}}-\mu)}} = -2\sum_{\vec{k}} \frac{1}{e^{\beta(\varepsilon_{\vec{k}}-\mu)} + 1} \\
&= -2\sum_{\vec{k}} f(\varepsilon_{\vec{k}}), \\
\frac{\partial^2\Phi_0}{\partial\mu^2} &= 2\sum_{\vec{k}} \frac{df}{d\varepsilon_{\vec{k}}} \quad \xrightarrow{T\to 0} \quad -2\rho_0(\varepsilon_F).
\end{aligned}$$

Then,

$$\boxed{\chi_{\text{Landau}} = -\frac{1}{3}\chi_{\text{Pauli}}}\,.$$

The total contribution of the conduction electrons to the susceptibility is

$$\boxed{\chi_{\text{total}} = \frac{2}{3}\chi_{\text{Pauli}}}\,,$$

and it is paramagnetic.

2.5 De Haas van Alphen effect

The de Haas van Alphen effect is the *periodic variation* of the magnetic susceptibility as a function of the inverse of the magnetic field. With this effect one can measure the Fermi surface of metals as well the effective mass of conduction electrons. The De Haas van Alphen effect is based on the energy quantization of the electrons due to the external magnetic field.

Let us consider the $k_x - k_y$ plane perpendicular to the magnetic field. Without application of a magnatic field, both k_x and k_y are good quantum numbers, *i. e.*, the electronic states are characterized through lattice points in the $k_x - k_y$ plane. In a magnetic field, the states are degenerate and characterized by the Landau quantum number n. There are

$$\frac{|e|BL_xL_y}{2\pi\hbar c}$$

degenerate states with energy $\hbar\omega_0(n+\frac{1}{2})$.

In order to understand quantum oscillations in the presence of a magnetic field, let us consider the two-dimensional free electron gas in the $x - y$ plane and a magnetic field applied along the z-direction. The Landau states are quantized and, since there is no third dimension, there is no continuum contribution. The energy eigenvalues are

$$E_n = \hbar\omega_0(n+\frac{1}{2}),$$

and the degeneracy for every level is

$$\frac{m\omega_0 L_xL_y}{2\pi\hbar} = \frac{|e|BL_xL_y}{2\pi\hbar c} = pB,$$

with

$$p = \frac{|e|BL_xL_y}{2\pi\hbar c}.$$

If we have a system of N electrons, pBn_0 electrons fill n_0 Landau levels, and the remaining $N - pBn_0$ electrons fill the $(n_0+1)^{\text{th}}$ level. The total energy is then given by

$$E_{\text{tot}} = \sum_{n=0}^{n_0-1} pB\hbar\omega_0(n+\frac{1}{2}) + \hbar\omega_0(N - pBn_0).$$

For larger B, the filling of the $(n_0+1)^{\text{th}}$ level decreases linearly. The situation is graphically expressed in Fig. 2.3.
If

$$B = \frac{N}{pn_0} \qquad \Rightarrow \qquad \boxed{\frac{1}{B} = \frac{pn_0}{N}},$$

the $(n_0+1)^{\text{th}}$ level won't be filled anymore, and the Fermi energy is then at the $n_0{}^{\text{th}}$ level. Therefore, for the total energy and magnetization we expect a $\frac{1}{B}$-periodic behavior.

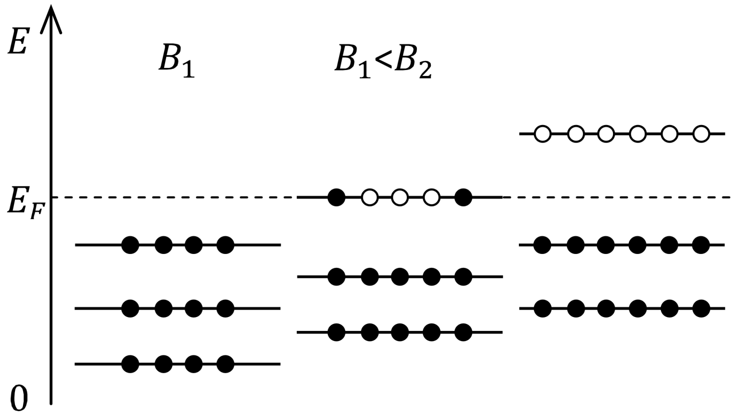


Abbildung 2.3: Filling of the Landau levels in different magnetic fields.

2.6 Quantum Hall effect

Since in two dimensions *only* discrete highly degenerate Landau levels are present, one can in such cases analyze the Landau quantization in detail. The density of states of a two-dimensional spinless non-interacting electron gas in a strong magnetic field is given by

$$\rho_{2\mathrm{d}}(E) = \frac{m\omega_0 L_x L_y}{2\pi\hbar} \sum_n \delta\left(E - \hbar\omega_0(n + \frac{1}{2})\right).$$

This density of states consists of delta peaks at the Landau energies $\hbar\omega_0(n + \frac{1}{2})$ weighted by the degeneracy.

With the help of semiconductor physics, it is possible to create a purely two-dimensional electron gas. This is done on heterostructures of p-doped GaAs and n-doped $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$. Using the molecular beam epitaxy (MBE) technique, one can grow alternately the two semiconductors in order to form a heterostructure. Each layer has a width of about several nanometers. $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ is n-type doped, which generates extra mobile electrons in its conduction band. These electrons migrate to fill the holes at the top of the GaAs valence band and partially end up as states near the bottom of the GaAs conduction band. There is of course a positive charge left on the donor impurities which attracts these electrons to the interface and "bends"the bands. This is the *source of electric field* in the system.

The transfer of electrons from $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ to GaAs continues until the dipole layer formed from the positive donors and the negative inversion layer is sufficiently strong. This dipole layer gives rise to a potential discontinuity, which makes the Fermi level of GaAs equal to that of $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$.
The electronic states perpendicular to the separation layer are localized so that in the layer between GaAs and $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ there is a two-dimensional electron gas.
A possible way to investigate this two-dimensional electron gas is by considering the Hall effect. For that we shall introduce this effect briefly.

Reminder: Hall effect.

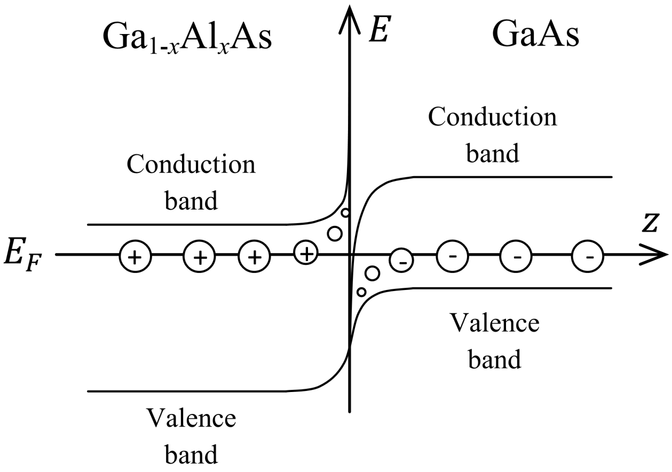


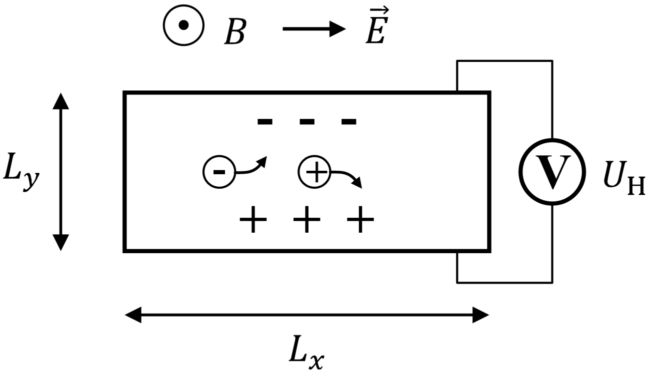
Abbildung 2.4: The scheme of the energy bands of the $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}/\mathrm{GaAs}$ heterostructure. The charge density of the system is $\sim 10^{11}$ cm^{-2}.

Under application of an electric field along the x-direction and a homogeneous magnetic field along the z-direction, the electrons in a conductor of length L_x and width L_y, moving at velocity v_x in the x-direction, feel a Lorentz force in the y-direction:

$$F_{\mathrm{L}} = \frac{e}{c} v_x B.$$

The charges bend in the y-direction until the created E_y-field compensates the Lorentz force:

$$E_y = \frac{v_x}{c} B = \frac{j_x B}{nec} = \frac{1}{nec} \frac{I}{L_y L_x} B = \frac{U_y}{L_y}.$$



Here, $U_y = U_\mathrm{H}$ is the Hall voltage, which is measured. It is determined by

$$U_\mathrm{H} = r_\mathrm{H} \frac{IB}{L_x}.$$

The proportionality coefficient r_{H},

$$\boxed{r_{\mathrm{H}} = \frac{1}{nec}},$$

is called the Hall coefficient and can be either positive or negative depending on whether the carriers are electrons or holes.

In the classical Hall effect, we have that the Hall resistance $\frac{U_{\mathrm{H}}}{I}$ is proportional to the magnetic field. In the two-dimensional electron system that we introduced, for large enough magnetic fields and low temperatures, this proportionality is not anymore fulfilled. In fact, what is observed is that the Hall resistivity ρ_{xy} shows steps and plateaux at quantized values of $\frac{h}{ie^2}$, where i is an integer. ρ_{xy} is not linear in B, but remains constant over a large interval of B and jumps at a critical B to the next quantized value $\frac{h}{(i-1)e^2}$ (see Fig. 2.5).

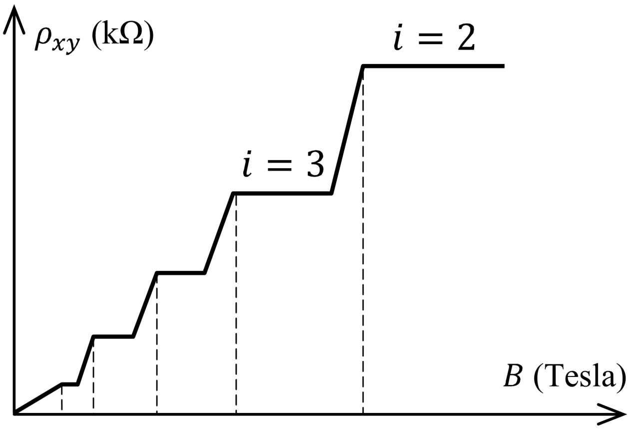


Abbildung 2.5: Schematic representation of the measured Hall resistance.

While the Hall resistivity shows quantized values, the longitudinal resistivity $\rho_{xx} = 0$.

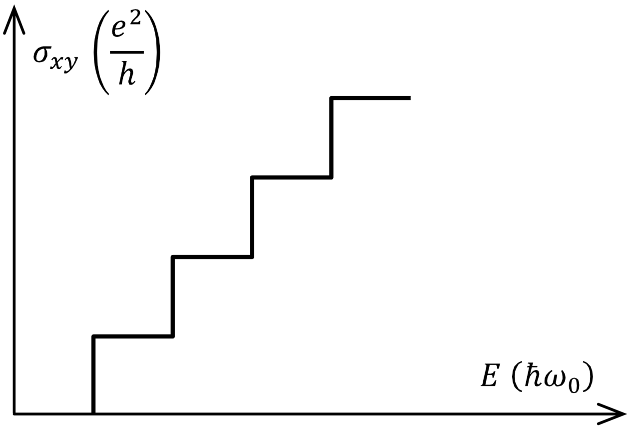
In the basis of the Landau states, the matrix elements of the current operator are given by

$$\begin{aligned}
\langle nk_y | j_x | lk'_y \rangle &= \frac{e}{m}\sqrt{\frac{m\hbar\omega_0}{2}}\left(\sqrt{n+1}\delta_{n,l-1} - \sqrt{n}\delta_{n,l+1}\right)\delta_{k_y k'_y}, \\
\langle nk_y | j_y | lk'_y \rangle &= -e\omega_0\sqrt{\frac{\hbar}{2m\omega_0}}\left(\sqrt{n+1}\delta_{n,l-1} + \sqrt{n}\delta_{n,l+1}\right)\delta_{k_y k'_y}.
\end{aligned}$$

Out of these matrix elements, one can derive the Hall conductivity:

$$\sigma_{xy} = \frac{e^2}{2\pi\hbar}(n+1) = \frac{e^2}{h}(n+1).$$

As a function of the Fermi energy, the Hall conductivity of the two-dimensional electron gas in a magnetic field follows a step-like behavior. The quantized values for the Hall conductivity are the values, where the Fermi energy falls in the gap between two discrete Landau levels.



There must be a mechanism that explains why the Fermi energy either remains in a gap between two Landau levels or in a region of occupied states and the current-carrying state does not change as a function of magnetic field.

Two-dimensional systems are not completely perfect, but have impurities and impurity scattering is possible. Through this impurity scatering and, in general, a disorder potential, the degeneracy of Landau levels is lifted and the Landau levels extend to Landau bands.

If the disorder is not very strong, there are still gaps between the Landau bands for various Landau values n. In every Landau band, there are delocalized states in the middle of the band, *i.e.*, where the original eigenvalue $\hbar\omega_0(n+\frac{1}{2})$ resided, and localized states at the boundaries of the Landau bands. The localized states do not contribute to the current transport, which means that when the Fermi energy is in the region of localized states the diagonal conductivity σ_{xx} disappears and the non-diagonal Hall conductivity σ_{xy} keeps the value that it takes in the gap between two Landau levels. Without disorder we cannot account for the plateau nature of the quantum Hall effect.

The observation that in the quantum Hall effect the quantization of the conductivity is an integer multiple of a universal constant means that this behavior can only be dependent on a very robust property of the two-dimensional systems: the geometry. The quantization of the conductivity is obtained in a one-dimensional channel. In the quantum Hall effect current arises from the states at the edge: EDGE STATES.

Up to now, we have talked about the *integer quantum Hall effect.* When the quality of samples is high enough, at low T and high B one observes non-integer steps:

$$\rho_{xy} = \frac{h}{fe^2},$$

with $f = \frac{p}{q}$ (p and q are integers, q is odd). In order to understand the fractional quantum Hall effect, one has to include electronic correlations. The excitations in such a system can be described through quasiparticles with non-integer charge. Laughlin won the Nobel Prize in 1998 for suggesting an ansatz wavefunction to describe the fractional quantum Hall effect.