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Contents

Chapter 1

Peierls Instability & Charge Order

1.1 Peierl Instability

link between peierls transition and lindhard screening `http://large.stanford.edu/courses/2008/ph373/yao1/`

Chapter 2

Linear Response Theory

2.1 From Causality to Kramer-Kronig relation

For a linear system to obey causality its response function has to have the following form

$$\tilde{\chi}(t) = \begin{cases} 0 & t < t_0 \\ \chi(t) & t > t_0 \end{cases} \tag{2.1}$$

This connection between the causality of a system and its response function can be exemplified in the following way. For a linear system, characterized by $\chi(t)$, the response to a input signal $x(t)$ is given as $y(t) = \int x(t-t')\chi(t')dt'$. By causality we understand that there can't be an effect which precedes its cause. Therefore we assume that $y(t_0)$ at particular time t_0 can only depend on the input signal $x(t)$ for $t \leq t_0$. In that sense we see that when writing $y(t)$ as

$$y(t) = \int_{-\infty}^{0} \chi(\tau)x(t-\tau)\, d\tau + \int_{0}^{\infty} \chi(\tau)x(t-\tau)\, d\tau \tag{2.2}$$

the first integral has to vanish. Since $x(t)$ is arbitrary, we can conclude that causality is only obeyed if $\chi(t) = 0$ for $t < 0$.

Like every analytical function we can split the response function $\hat{\chi}(t)$ in an even $\chi_{\text{even}}(t)$ and an odd $\chi_{\text{odd}}(t)$ part

$$\tilde{\chi}(t) = \frac{\tilde{\chi}(t) + \tilde{\chi}(-t)}{2} + \frac{\tilde{\chi}(t) - \tilde{\chi}(-t)}{2} = \chi_{\text{even}}(t) + \chi_{\text{odd}}(t) \tag{2.3}$$

Multiplying the even part of this function with the signum function yields,

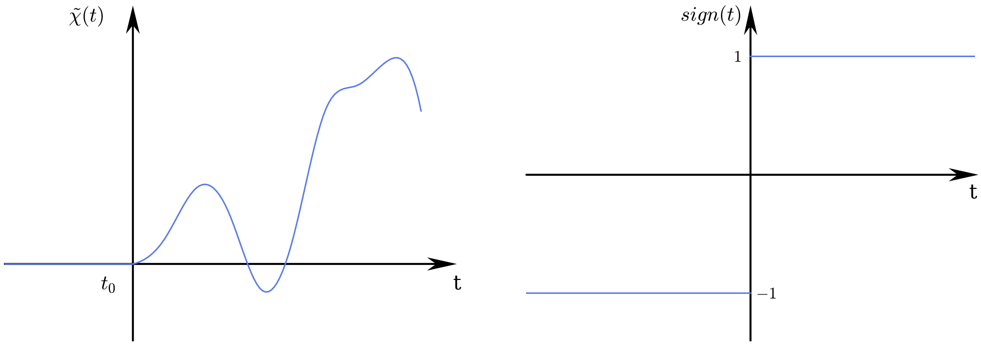

Figure 2.1: Left: An example of a response function obeying causality as stated by Eq 2.1 . **Right:** Graphical illustration of the sign function.

$$\text{sign}(t)\cdot\chi_{\text{even}} = \text{sign}(t)\cdot\left\{\frac{\tilde{\chi}(t)}{2}+\frac{\tilde{\chi}(-t)}{2}\right\} = \frac{\tilde{\chi}(t)}{2}-\frac{\tilde{\chi}(-t)}{2} = \chi_{\text{odd}}(t) \tag{2.4}$$

Using this relation to replace $\chi_{\text{odd}}(t)$ in Eq 2.3 gives

$$\tilde{\chi}(t) = \chi_{\text{even}}+\chi_{\text{odd}} = \underbrace{(1+\text{sign}(t))}_{\text{step function}}\cdot\chi_{\text{even}}(t) = 2\sigma(t)\cdot\chi_{\text{even}}(t) \tag{2.5}$$

Taking into account that the Fourier transformation conserves the symmetry of a function, by transforming the real and odd function $\chi_{\text{odd}}(t)$ we get a imaginary and odd function $\chi_{\bullet}textodd(\omega)$.

$$\begin{aligned}\chi_{\text{odd}}(\omega) &= \int \chi_{\text{odd}}(t)\cdot e^{i\omega t}\,dt = \int_{-\infty}^{\infty}\chi_{\text{odd}}(t)\cdot\{\underbrace{\cos(\omega t)}_{\text{even}}+i\underbrace{\sin(\omega t)}_{\text{odd}}\}\,dt \\ &= i\int_{-\infty}^{\infty}\chi_{\text{odd}}(t)\cdot\sin(\omega t)\,dt = i\chi''(\omega) \end{aligned}\tag{2.6}$$

To get to this result we also used the fact that the integral over the entire range vanished for an odd integrand.

Example: Damped Harmonic Oscillator

The differential equation of a driven damped harmonic oscillation is given as

$$\ddot{x}(t) + \gamma\dot{x}(t) + \omega_0^2 x(t) = f(t) \tag{2.7}$$

where γ is the damping coefficient and ω_0 is the resonance frequency. The solution to this differential equation can be found rather easy by transforming it to the Fourier space.

$$-\omega^2 x(\omega) \;-\; i\omega\gamma x(\omega) \;+\; \omega_0^2 x(\omega) \;=\; f(\omega) \tag{2.8}$$

We define the systems response function in Fourier space as

$$\chi(\omega) \;\equiv\; \frac{x(\omega)}{f(\omega)} \;=\; \frac{1}{\omega_0^2 - \omega^2 + i\gamma\omega} \;=\; |\chi(\omega)|\{\cos(\phi) + i\sin(\phi)\} \tag{2.9}$$

The benefit of doing so lays in the fact, that $\chi(\omega)$ depends solely on the system specific quantities like the resonance frequency ω_0 and the damping coefficient γ.

In that sense the response function is characteristic to your system and doesn't depend on the applied driving force $f(\omega)$. This is handy because as soon as we have determined $\chi(\omega)$ for a given system, we can find the Fourier transform of the solution to Eq 2.7 for various driving forces by just multiplying the Fourier transforms of the response function and the driving force

$$x(\omega) \;=\; \chi(\omega)\cdot f(\omega) \;=\; f(\omega)|\chi(\omega)|\{\cos(\phi(\omega)) + i\sin(\phi(\omega))\} \tag{2.10}$$

on the left side we described the response function in terms of its magnitude $|\chi(\omega)|$ and its frequency dependent phase $\phi(\omega)$.

Splitting the response function up in a real and imaginary part we get

$$\mathrm{Re}\;\chi(\omega) \;\equiv\; \chi'(\omega) \;=\; \frac{\omega_0^2 - \omega}{(\omega^2 - \omega_0^2)^2 + \omega^2\gamma^2} \tag{2.11}$$

$$\mathrm{Im}\;\chi(\omega) \;\equiv\; \chi''(\omega) \;=\; \frac{-\gamma\omega}{(\omega^2 - \omega_0^2)^2 + \omega^2\gamma^2} \tag{2.12}$$

To illustrate that this solution is correct, we look at the special case were the driving force is a harmonic oscillation

$$f(t) \;=\; f_0\cos(\omega_0 t) \quad\Rightarrow\quad f(\omega) \;=\; f_0\left(\delta(\omega_0 - \omega) + \delta(\omega_0 + \omega)\right) \tag{2.13}$$

As an ansatz for a solution to Eq 2.7 we choose

$$x(t) \;=\; f_0|\chi(\omega)|\cos(\omega t) \tag{2.14}$$

We check if this ansatz is correct by calculating its Fourier transform. Using

$$\int \cos(\omega_0 t)\; e^{i\omega t}\; dt \;=\; \int \frac{e^{i\omega_0 t} + e^{-i\omega_0 t)}}{2}\; e^{i\omega t}\; dt \;=\; \frac{1}{2}\int e^{i(\omega+\omega_0)t} + e^{i(\omega-\omega_0)t}\; dt$$
$$= \frac{1}{2}\delta(\omega+\omega_0) \;+\; \delta(\omega-\omega_0) \qquad (2.15)$$

we get

$$x(\omega) \;=\; \frac{f_0|\chi(\omega)|}{2}(\delta(\omega+\omega_0) \;+\; \delta(\omega-\omega_0)) \qquad (2.16)$$

Power consumption due to the velocity dependent damping term in Eq 2.7 is given as

$$\begin{aligned} P(t) &= f(t)\cdot\dot{x}(t) \;=\; f_0^2\;|\chi(\omega)|\;(-\omega)\;\cos(\omega t)\sin(\omega t-\phi) \\ &= -f_0^2\;|\chi(\omega)|\;\omega\;\left[\cos(\omega t)\sin(\omega t)\cos(\phi) - \cos^2(\omega t)\sin(\phi)\right] \qquad (2.17)\end{aligned}$$

We are interested in the time averaged power dissipated due to the damping term

$$\begin{aligned} \langle P\rangle &= \frac{1}{T}\int_0^T P(t)\; dt \\ &= \frac{f_0^2}{T}\;|\chi(\omega)|\;\omega\;\int_0^T \cos(\omega t)\sin(\omega t)\cos(\phi) - \cos^2(\omega t)\sin(\phi)\; dt \\ &= \frac{f_0^2}{2}\;|\chi(\omega)|\;\omega_0\sin(\phi) \;=\; \frac{f_0^2}{2}\;\omega_0\;\chi''(\omega_0) \qquad (2.18)\end{aligned}$$

To get to this result we used the properties $\int_0^T \cos(\omega t)\sin(\omega t)\; dt = 0$ and $\int_0^T \cos^2(\omega t)\; dt = 1/2$ of the trigonometric functions when integrating over one period T. We further replaced the period with the frequency ω_0 by using $T = 2\pi/\omega_0$. Using the polar form of the susceptibility introduced in Eq 2.9 we can assign the average power loss to the imaginary part $\chi''(t)$.

The physical implication here is that, seen at the example of the damped harmonic oscillator, the dissipated energy of a system can be linked to the imaginary part of its response function. This is interesting because it allows us to evaluate the energy put through (dissipated in) a system by just looking at the the response functions real (imaginary) part in the frequency domain. It is also nice to see that the very physical distinction between energy transmission and dissipation can be recognized again in a purely mathematical property, as the real- and imaginary part, of a systems characterizing quantity like the susceptibility.

Kramers-Kronig Relation

$$i\chi''(\omega) \;=\; \chi_{\text{odd}}(\omega) \;=\; \int \text{sign}(t)\cdot\chi_{\text{even}}(t)e^{i\omega t}\;dt \;=\; \mathcal{FT}\{\text{sign}(t)\} * \mathcal{FT}\{\chi_{\text{even}}(t)\} \quad (2.19)$$

to write the convolution of the Fourier transforms the convolution theorem was used. Before evaluating the convolution we compute the Fourier transform of the sign function. Since sign(t) is an odd function its Fourier transform can be written as

$$\int \text{sign}(t)\sin(\omega t)\;dt \;=\; 2i\int_0^{\pi/\omega}\sin(\omega t)\;dt \;=\; \frac{2i}{\omega} \quad (2.20)$$

Given by the periodicity of the sine function the integration over the range $t \in \mathbb{R}/[-\pi/\omega, \pi/\omega]$ cancels out. Furthermore since the integrand is even we only have to integrate from 0 to π/ω. The discontinuity introduced by the ω^{-1} term is due to the sign function and and has no physical origin. Plugging sign(ω) into Eq 2.19 leads to

$$i\chi''(\omega) \;=\; \int_{-\infty}^{\infty}\text{sign}(\omega'-\omega)\;\chi'(\omega')\;d\omega' \;=\; \mathcal{P}\int_{-\infty}^{\infty}\frac{2i}{\omega'-\omega}\;\chi'(\omega')\;d\omega' \quad (2.21)$$

The imaginary unit i is present on both sides of the equation therefore we neglect it

$$\begin{aligned}\chi''(\omega) \;&=\; 2\mathcal{P}\int_{-\infty}^{\infty}\frac{\chi'(\omega)}{\omega'-\omega}\;d\omega' \;=\; 2\mathcal{P}\int_{-\infty}^{\infty}\frac{\chi''(\omega')(\omega'+\omega)}{(\omega'^2-\omega^2)}\;d\omega' \\ &=\; 2\mathcal{P}\int_{-\infty}^{\infty}\frac{\omega\;\chi'(\omega')}{\omega'^2-\omega^2}\;d\omega' \end{aligned} \quad (2.22)$$

in the last step we used the fact that the integration $\omega'\chi'(\omega')$ cancels out since the integrand is odd. This relation is between $\chi''(\omega)$ and $\chi'(\omega)$ is known as the **Kramers-Kronig Relation**. It is a direct consequence of the causality of the response function (Eq 2.1).

Further Examples of Response Functions

From Ohm's law we know, that the current density $\mathbf{j}$ in a material is related to the electric field $\mathbf{E}$ in the material by the equation $\mathbf{j} = \sigma\mathbf{E}$ where σ is the material dependent electrical conductivity. Ohm's Law is mostly used for the static case. In the more general case were we assume that the current density and the electric field have a frequency dependent component, we can generalize Ohm's law with the help of linear response theory to become

$$\mathbf{j}(\omega) \;=\; \sigma(\omega)\mathbf{E}(\sigma) \quad (2.23)$$

in this case we refer to $\sigma(\omega)$ as the optical conductivity[1].

[1] Wikipedia - Optical conductivity - `https://en.wikipedia.org/wiki/Optical_conductivity`

For experiments it's useful to define the electric displacement field $\mathbf{D}(t)$. Its Fourier transform is given as

$$\mathbf{D}(\omega) \quad = \quad \varepsilon(\omega)\mathbf{E}(\omega) \tag{2.24}$$

with the dielectric function $\varepsilon(\omega)$ as the response function of the system. This function is composed of

$$\varepsilon(\omega) \quad = \quad \varepsilon_0 \; + \; \frac{i}{2}\sigma(\omega) \tag{2.25}$$

The dielectric function can be linked to the refraction index of a material by

$$\sqrt{\varepsilon(\omega)} \quad = \quad n(\omega) \quad = \quad n'(\omega) \; + \; in''(\omega) \tag{2.26}$$

Looking at the special case where the incident angle is zero $\vartheta = 0$ and therefore the wave vectors $\mathbf{k}_i$, $\mathbf{k}_r$ and $\mathbf{k}_t$ of the incident, reflected and transmitted plane waves lay on one line perpendicular to the surface. We can write for the incident $\mathbf{E}_i$ and transmitted $\mathbf{E}_t$ electric field component as

$$\begin{gathered} \mathbf{E}_i \propto e^{i(\mathbf{k}_i z - \omega t)} \;, \\ \mathbf{E}_t \propto e^{i(\mathbf{k}_t z - \omega t)} \quad \Rightarrow \quad \mathbf{E}_t \propto e^{i\{(n' + in'')\mathbf{k}_i z - \omega t\}} = e^{-n''\mathbf{k}_i z} \; e^{i(n'\mathbf{k}_i z - \omega t)} \end{gathered} \tag{2.27}$$

By introducing $\lambda = 1/\mathbf{k}_i n''$ we get for the transmitted electric field

$$\mathbf{E}_t \propto e^{-z/\lambda} \; e^{i(n'\mathbf{k}_i z - \omega t)} \tag{2.28}$$

In reflection measurements the accessible quantity is the reflectivity $R(\omega)$

$$R(\omega) \quad = \quad \left|\frac{1-n}{1+n}\right|^2 \quad = \quad \left|\frac{1 - n'(\omega) - in''(\omega)}{1 + n' + in''}\right|^2 \tag{2.29}$$

By measuring the reflectivity one can compute only the real part $n'(\omega)$ of the refractive index since the phase information is lost because of the quadratic dependence. But if $n'(\omega)$ over a large frequency range one can compute the imaginary part $n''(\omega)$ by applying Kramers-Kronig Relation. Doing that allows then to reconstruct the complete refractive index $n(\omega)$. If the refractive index is known it isn't difficult to compute then material specific quantities like the dielectric function $\varepsilon(\omega)$ or the optical conductivity $\sigma(\omega)$.

Chapter 3

Quantum Oscillations & ARPES

3.1 Quantum Oscillations

3.1.1 Landau Cylinder

Charged particles exposed to a magnetic field B are forced to move on closed circles on which they have a quantized energy. For free electrons in a magnetic field along the z-axis this energy can be written as

$$E = \left(n + \frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2}{2m}k_z^2 \quad (3.1)$$

This quantization of accessible states in reciprocal space is illustrated in Fig.3.1 . The electrons are free to move along the corresponding axes in reciprocal space along which the magnetic field is applied. In the plane (in **k**-space) perpendicular to the magnetic field, the energy states lie on circles (Fig.3.1 right, bottom). This restriction lead to the characteristic picture of the nested cylinders (left image in Fig.3.1). These cylinders are called **Landau cylinders** and the energy scale of quantization of the radius of these cylinders is given by the **cyclotron frequency** $\omega_c = eB/m$.

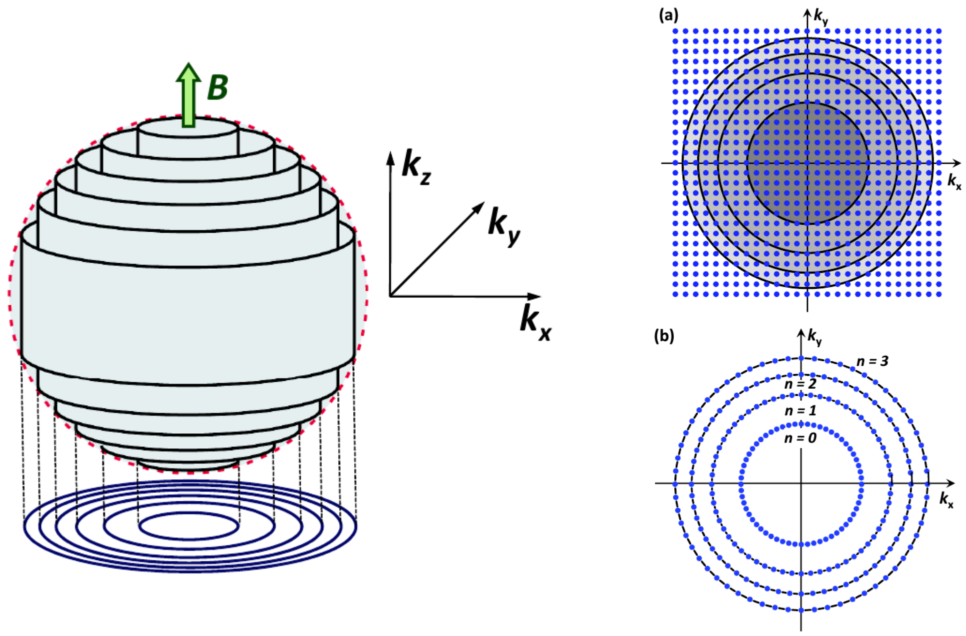

Figure 3.1: **left**: Occupied states in reciprocal space of a free electron gas in a magnetic field. The accessible energy states are inside the sphere bound to lay on cylinders with radius $\mathbf{k}_\perp = \sqrt{(n+1/2)2m\omega_c/\hbar}$. **right**: top sketch shows accessible states of electrons in a plane in reciprocal space for $B = 0$. Bottom picture shows accessible states now arranged in circles due to $B \neq 0$.

3.1.2 Onsager Relation

Starting from the Landau quantization condition, it can be shown that the surface in reciprocal space s_n enclosed by the n-th cylinder can be linked to the magnetic field B

$$S_n = (n+\gamma)\frac{2\pi e}{\hbar}B \tag{3.2}$$

here γ is a correction term which would become important by a more detailed analysis. Since this term cancels out later we don't elaborate it further.

Experimentally accessible for us are the B-field dependent oscillations of macroscopic quantities like resistivity and magnetization. These oscillations are caused by the variation of the number of electrons right at the Fermi surface due to the fact, that with increasing magnetic field the landau cylinders are pushed across the Fermi surface. Looking at the situation were the surface of the $n+1$-th Landau cylinder is equal to the Fermi surface S_F, we have a maximal electron concentration. We refer to the applied field in this condition as B_{n+1}. Increasing the magnetic field will reduce the electron concentration again until the electrons distributed over the n-th landau cylinder coming in proximity of the Fermi surface and start to populate it. The electron concentration becomes then maximal again, at the magnetic field B_n, when the surface of the n-th Landau cylinder matches the Fermi surface ($S_n = S_F$). We can express these conditions in the following equations

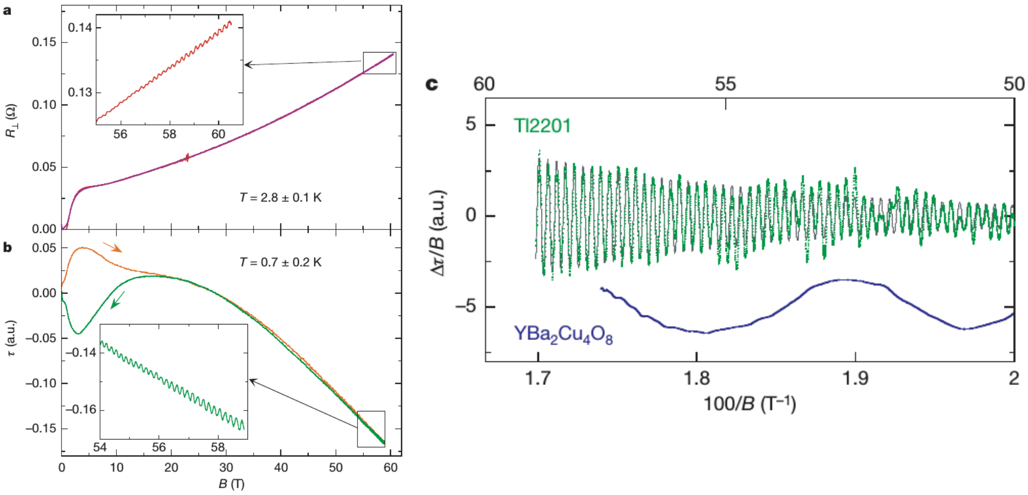

Figure 3.2: **a.** and **b.** show quantum oscillation measurements data on resistivity and magnetic torque. Oscillations of the measured quantities are clearly visible in the graphs inset. **c.** Oscillatory component of the data from b plotted over $1/B$. Figures are adapted from [5].

$$S_{n+1} \quad = \quad (n+1+\gamma)\frac{2\pi e}{\hbar}B_{n+1}, \qquad S_n \quad = \quad (n+\gamma)\frac{2\pi e}{\hbar}B_n \tag{3.3}$$

Since we assume that $S_{n+1} = S_n = S_F$, we can relate the Fermi surface to the change in magnetic field

$$\left(\frac{1}{B_{n+1}} - \frac{1}{B_n}\right) \quad = \quad \Delta\left(\frac{1}{B}\right) \quad = \quad \frac{2\pi e}{\hbar S_F} \tag{3.4}$$

$\Delta(1/B)$ can be understood as the period of the oscillation when plotting the measured quantity over $1/B$. In practice it is more convenient to define the frequency F with which the inverse magnetic field oscillates $F = (\Delta(1/B))^{-1}$ which has the units of Tesla. Expressing Eq 3.4 in terms of the frequency we get the **Onsager Relation**

$$F \quad = \quad \frac{\hbar}{2\pi e}S_F \tag{3.5}$$

Typical measurement data are shown in Fig.3.2 . Once the oscillatory component of the raw measurement data is extracted one can perform a Fourier transformation to determine the frequency F from which then the Fermi surface can be calculated (Fig.3.3).

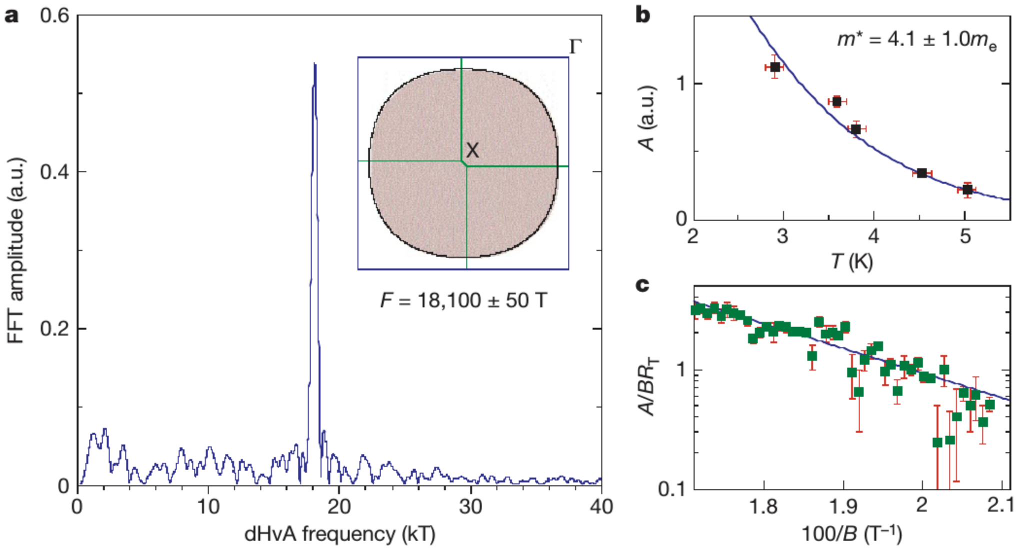

Figure 3.3: **a.** Fourier transformation of the measurement data displayed in Fig.3.2 . The oscillation frequency can easily deduced from here to be around 18 kT. **b.** shows the temperature dependence of the oscillation amplitude. From this the effective electron mass m^* can be calculated, using the Lifshitz-Kosevich formula. **c.** displays the decay of the oscillation amplitude in respect to the inverse magnetic field. This is also visible in subplot c. in Fig.3.2 . From this the electron mean free path can be calculated. From [5].

Effective mass and Mean Free Path

Using the Lifshitz-Kosevich Formula[1] further conclusion on the electrons effective mass m^* and mean free path λ_{mfp} can be drawn from the above measurement results. By measuring the oscillations amplitudes temperature dependence one can calculate the electrons effective mass at the Fermi surface (Fig.3.2 .b.).

Visible in Fig.3.2 .c. we see a decay of the oscillation amplitude for going to lower magnetic fields. This can be described with the following formula

$$\Delta\tau/B \quad \propto \quad e^{\left(-\frac{\pi\hbar k_F}{eBl}\right)} \tag{3.6}$$

where l is the mean free path of the electrons in the material. Estimating the maximal amplitudes and plot it in a semi log plot over $1/B$ allows then to estimate l from the straight line slope. This is done in Fig.3.3 .c.

[1] Derivation can be found in chapter two of *Magnetic oscillations in Metal* from D. Schoenberg [4]. More descriptive explanation can be found in the caption of figure 6. in [3].

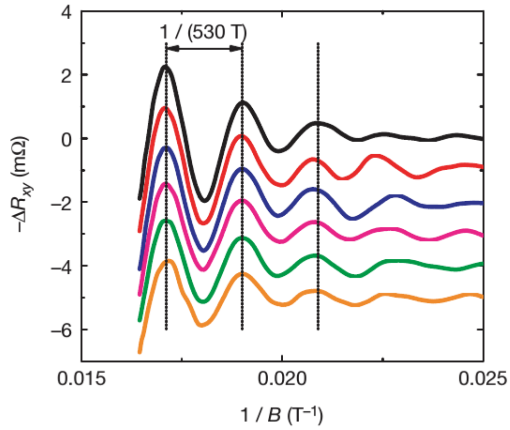

Figure 3.4: Oscillatory part of the Hall resistivity at different temperature. The oscillation amplitude reduces with increasing temperature whereas the frequency stays constant. From [1].

De Haas-van Alphen effect and Shubnikov-de Hass effect

If we measure oscillations in the magnetization of a material we refer to it as the **de Haas-van Alphen effect**. Typical measurements are displayed in Fig.3.2 .b where the magnetically induced torque τ on a sample is used to measure the samples magnetization. The link between the variation of electron concentration at the Fermi surface and the oscillation of the magnetization can be exemplified in the following way: with changing electron concentration the inner energy also changes. With the help of thermodynamics we can see, that a oscillation inner Energy U should also lead to a oscillating magnetization.

Observing oscillations in the electrical resistivity ρ of a material is referred to as the **Shubnikov-de Hass effect** (Fig.3.2 .a and Fig.3.4). Finding a explanation to link to the oscillation resistivity of varying electron concentration at the Fermi surface is more difficult since there is no thermodynamical relation between the inner energy and the resistivity. On way of exemplifying this is that the scattering probability (and therefor the resistivity) is proportional to the density of states at the Fermi level. A oscillation in the DOS leads therefore in an oscillating resistivity.

3.2 Angle Resolved Photo Emission Spectroscopy

3.2.1 Scattering Experiment

sketch scattering experiment

3.2.2 Fermi's Golder Rule

$$W \propto |\langle \mathbf{k}_f | V(\mathbf{r}) | \mathbf{k}_i \rangle|^2 \tag{3.7}$$

3.2.3 Angle Resolved Photo Emission spectroscopy

adapt ARPES section from BA

Chapter 4

Second Quantization

4.1 1D-Chain of Atoms

To have a first insight into second quantization, we look at a phonons emerging in a one dimensional chain of atoms

skech 1D lattice chain

In the sketch above u_i refers to the distance from equilibrium of the i-th atom, p_i stands for the momentum of the i-th atom, K is the spring constant and the lattice constant a. The Hamiltonian of this system is given as

$$H_{\text{ph}} = \sum_{j_1}^{N} \left\{ \frac{1}{2M} p_j^2 + \frac{1}{2} K (u_j - u_{j-1})^2 \right\} \tag{4.1}$$

Since our problem has one dimension in real space it has also one dimension in the reciprocal space. We can introduce two length scales in the reciprocal space

1. The size of the one dim. unit cell defines the length of the reciprocal lattice vector $\vec{G}$ which is equal to the size of the Brillouin zone: $G = 2\pi/a$
2. The length L of the chain of atoms in real space defines the lowest possible distance two points in reciprocal space can have $\Delta k_{\text{min}} = 2\pi/L$.

sketch 1D k-space

We now want to rewrite the Hamiltonian Eq 4.1 by replacing the distance from equilibrium and the momentum of the atoms by its Fourier transformations

$$p_j \;=\; \frac{1}{\sqrt{N}} \sum_{k \in \mathrm{BZ}} P_k e^{ikR_j^0} \qquad \Longleftrightarrow \qquad P_k \;=\; \frac{1}{\sqrt{N}} \sum_j p_j e^{-ikR_j^0} \tag{4.2}$$

$$u_j \;=\; \frac{1}{\sqrt{N}} \sum_{k \in \mathrm{BZ}} U_k e^{ikR_j^0} \qquad \Longleftrightarrow \qquad U_k \;=\; \frac{1}{\sqrt{N}} \sum_j u_j e^{-ikR_j^0} \tag{4.3}$$

Since it is a cumbersome procedure we look at the calculate the different terms from Eq 4.1 separately. We start with $\sum_i p_j^2$:

$$p_j \;=\; \frac{1}{\sqrt{N}} \sum_k P_k e^{ikR_j^0} \;=\; \frac{1}{2\sqrt{N}} \left\{ \underbrace{\sum_k P_k e^{ikR_j^0}}_{\mathrm{A}} + \underbrace{\sum_{-k} P_{-k} e^{-ikR_j^0}}_{\mathrm{B}} \right\} \tag{4.4}$$

The second equality sign holds because summing two times and sum and dividing by two gives the same result. Additionally in the second sum we replaced $k \to -k$. No we can write

$$\begin{aligned} p_j^2 \;&=\; \frac{1}{4N} \left(A^2 \;+\; B^2 \;+\; 2AB\right) \;=\; \frac{2}{4N} \sum_j AB \\ &=\; \frac{1}{2N} \sum_j \sum_k \sum_{-k} P_k P_{-k} \;=\; \sum_k P_k P_{-k} \end{aligned} \tag{4.5}$$

is this correct?

To get to this result $\sum_j = e^{ikR_j^0} = \delta(k)$ was used. For evaluating now $\sum_j (u_j - u_{j-1})^2$ we use

$$u_j \;=\; \left\{ \underbrace{\sum_k u_k e^{ikR_j^0}}_{\mathrm{A'}} + \underbrace{\sum_{-k} u_{-k} e^{-ikR_j^0}}_{\mathrm{B'}} \right\} \tag{4.6}$$

$$\begin{aligned} u_{j-1} \;&=\; \frac{1}{\sqrt{N}} \sum_k u_k e^{ikR_j^0} e^{-ika} \\ &=\; \frac{1}{2\sqrt{N}} \left\{ \sum_k u_k e^{ikR_j^0} e^{-ika} \;+\; \sum_{-k} u_{-k} e^{-ikR_j^0} e^{ika} \right\} \end{aligned} \tag{4.7}$$

To get the final expression for u_{j-1} we used $R_{j-1}^0 = r_j^0 - a$.

$$
\begin{aligned}
\sum_j (u_j \; - \; u_{j-i})^2 \;\; &= \;\; \sum_j (u_j^2 \; + \; u_{j-1}^2 \; + \; 2u_j u_{j-1}) \\
&= \;\; \sum_k \left\{ u_k u_{-k} \; + \; u_k u_{-k} \; - \; 2u_k u_{-k} \frac{e^{-ika} \; + \; e^{ika}}{2} \right\} \\
&= \;\; \sum_k 2u_k u_{-k} \left\{ 1 \; - \; \cos(ka) \right\} \\
&= \;\; \sum_k 2u_k u_{-k} \sin^2(ka/2)
\end{aligned} \tag{4.8}
$$

In the step were the summing over j changed to a summing over k the same arguments as for Eq 4.5 were used. As we already know from the *introduction to solid state physics* class, we can assign the argument of the sum in the final expression as the square of the phonon dispersion relation $\omega(k)$

$$
\omega(k) \;\; = \;\; \omega_k \;\; = \;\; \sqrt{\frac{2K}{M}(1 - \cos(ka)} \;\; = \;\; \sqrt{\frac{4K}{M}} |\sin(ka/2)| \tag{4.9}
$$

Plugging our solutions for $\sum_j p_j^2$ and $\sum_j (u_j - u_{j-1})^2$ into Eq 4.1 yields

$$
H_{\mathrm{ph}} \;\; = \;\; \sum_{j=1}^{N} \left\{ \frac{1}{2M} P_k P_{-k} \; + \; \frac{M\omega_k^2}{2} u_k u_{-k} \right\} \tag{4.10}
$$

This expression similar to the Hamiltonian from the harmonic oscillator. We therefore define the latter operators b_k and $b_k^\dagger$

$$
b_k \;\; = \;\; \frac{1}{\sqrt{2}} \left(\frac{u_k}{l_k} \; + \; i \frac{p_k}{\hbar / l_k} \right) \tag{4.11}
$$

$$
b_k^\dagger \;\; = \;\; \frac{1}{\sqrt{2}} \left(\frac{u_k}{l_k} \; - \; i \frac{p_k}{\hbar / l_k} \right) \tag{4.12}
$$

and rewrite H_{ph} as

$$
H_{\mathrm{ph}} \;\; = \;\; \sum_k \hbar\omega_k (b_k^\dagger b_k \; + \; 1) \tag{4.13}
$$

This analogy between the Hamiltonian from the harmonic oscillations and Eq 4.10 emphasis that we can describe the state if excited phonons in a solid as a combination of different modes similar to the different modes of oscillations of an excited harmonic oscillator. Further we can use the latter operators applied to the vacuum state to describe the excited states mathematically.

picture single atom phonon dispersion relation picture two atom basis phonon dispersion relation ...if going down in temperature Peierls transition occurs -¿ Kohn anomaly

why is neutron scattering good for probing acoustic bands? - check lecture notes for explanation

...neutrons only probe lattice and neglect electronic structure

This way of describing the physical processes in terms of latter operators can be extended much more. It turns out that it is a very convenient way of describing physical problems and is used broadly in various fields in condensed matter physics. In the next sections we will learn how to apply this formalism more generally.

4.2 Free electron gas

Hamiltonian of a free electron gas can be written as.

$$H = \sum_{k\sigma} \frac{(\hbar \mathbf{k})^2}{2m} c^\dagger_{k\sigma} c_{k\sigma} \tag{4.14}$$

The ground state at $T = 0K$ is created by applying the electron-creation operators $c_{k_i\uparrow}$ of the $i-$th electron to the vacuum state $|0\rangle$ for every electron that is present in the electron gas.

$$|\mathrm{FS}\rangle = c_{k_{N/2}\uparrow} c_{k_{N/2}\downarrow} ... c_{k_1\uparrow} c_{k_1\downarrow} |0\rangle \tag{4.15}$$

To get the total number of electrons N the number operator $\hat{N} = \sum_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma}$ can be applied on the ground state $|\mathrm{FS}\rangle$

$$N = \langle \mathrm{FS}|\hat{N}|\mathrm{FS}\rangle = \langle \mathrm{FS}| \sum_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma} |\mathrm{FS}\rangle \tag{4.16}$$

Since we consider a free electron gas in its ground state at $T = 0K$ the momentum values $\mathbf{k}$ are limited to lay inside a sphere with radius k_F. Furthermore we have to take into account that in the system under consideration the orientation of the spin σ doesn't matter. Therefore we can replace the sum $\sum_\sigma$ by a factor two.

$$\begin{aligned} N &= \sum_{\mathbf{k}\sigma} \langle \mathrm{FS}|c^\dagger_{k\sigma} c_{k\sigma}|\mathrm{FS}\rangle = 2 \sum_{|\mathbf{k}| \;\leq k_F} \langle \mathrm{FS}|\mathrm{FS}\rangle = 2V \int \frac{d^3k}{(2\pi)^3} \theta(k_F - |\mathbf{k}|) \langle \mathrm{FS}|\mathrm{FS}\rangle \\ &= \frac{2V}{(2\pi)^3} \int\limits_{|\mathbf{k}| \leq k_F} d^3k \end{aligned} \tag{4.17}$$

Solving this integral in spherical coordinates gives

$$N = \frac{2V}{(2\pi)^3}\int_0^{k_F} dkk^2 \int_{-1}^{1} d\cos(\vartheta)\int_0^{2\pi} d\phi = \frac{1}{3}\frac{V}{\pi^2}k_F^3 \tag{4.18}$$

From that equation we can determine the electron density n for a three dimensional free electron gas at zero Temperature

$$n = N/V = k_F^3/(3\pi^2) \tag{4.19}$$

As another example of the usage of second quantization we want to determine now the ground state energy E_0 of the free electron gas

$$\begin{aligned} E_0 &= \langle \mathrm{FS}|H|\mathrm{FS}\rangle = \sum_{\mathbf{k}\sigma}\frac{\hbar\mathbf{k})^2}{2m}\langle \mathrm{FS}|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|\mathrm{FS}\rangle = \frac{\hbar^2}{2m}\sum_{\mathbf{k}\sigma}k^2\theta(|\mathbf{k}|-k_F) \\ &= 2\frac{4\pi V}{(2\pi)^3}\frac{\hbar^2}{2m}\int dk\theta(|\mathbf{k}|-k_F)k^4 \\ &= \frac{4\pi V}{(2\pi)^3}\frac{\hbar}{m}\frac{k_F^5}{5} = \frac{3}{5}NE_F \end{aligned} \tag{4.20}$$

To get to the final expression we used the electron density from Eq 4.19 and the Fermi Energy $E_F = (\hbar k_F)^2/(2m)$.

4.3 Electron-Electron Interaction

The electron-electron interaction term in a material is given as

$$V_{\text{el-el}} = \frac{1}{2V}\sum_{\sigma_1,\sigma_2}\sum_{k_1,k_2,q} V_q c^\dagger_{k_1,\sigma_1}c^\dagger_{k_2,\sigma_2}c_{k_1+q,\sigma_1}, c_{k_2-q,\sigma_2} \tag{4.21}$$

To understand this expression better we look first at one single interaction between two electrons with initial momentum and spin k_1, σ_1 and k_2, σ_2. The spin doesn't change. When colliding the exchanged momentum due to the interaction term V_q, were we assume $q \neq 0$. The electron momenta in the final state are related by $k_1 + q = k_2$.

The interaction is due to the coulomb repulsion, therefore we can write the interaction term in reciprocal space as

$$V_q = \int d^3re^{i\mathbf{q}\cdot\mathbf{r}}V(\mathbf{r}) = \int d^3r\frac{e^2}{r}e^{i\mathbf{q}\cdot\mathbf{r}} = \frac{4\pi e^2}{q^2} \tag{4.22}$$

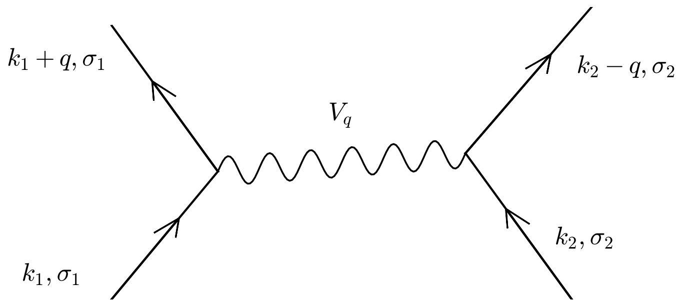

Figure 4.1: illustration of an e-e Interaction were the incoming electrons have initial momentum k_1, k_2 and spin σ_1, σ_2. The interaction V_q causes them to exchange a momentum q.

Calculating the change in energy resulting from the coulomb interaction between the electrons gives

$$\frac{E_1}{N} = \frac{\langle \mathrm{FS}|V_{\text{el-el}}|\mathrm{FS}\rangle}{N} = \frac{1}{2VN}\sum_q \sum_{\mathbf{k}_1,\mathbf{k}_2}\sum_{\sigma_1,\sigma_2}\frac{4\pi^2}{q^2}\langle \mathrm{FS}|c^\dagger_{\mathbf{k}_1+q}c^\dagger_{\mathbf{k}_2-q}c_{\mathbf{k}_2}c_{\mathbf{k}_1}|\mathrm{FS}\rangle \qquad (4.23)$$

$$\begin{aligned}\langle \mathrm{FS}|c^\dagger_{\mathbf{k}_1+q,\sigma_1}c^\dagger_{\mathbf{k}_2-q,\sigma_2}c_{\mathbf{k}_2,\sigma_2}c_{\mathbf{k}_1,\sigma_2}|\mathrm{FS}\rangle &= \delta_{\sigma_1\sigma_2}\delta_{\mathbf{k}_1+q,\mathbf{k}_2}\langle \mathrm{FS}|c^\dagger_{\mathbf{k}_1+q}c^\dagger_{\mathbf{k}_2-q}c_{\mathbf{k}_2}c_{\mathbf{k}_1}|\mathrm{FS}\rangle \\ &= -\delta_{\sigma_1\sigma_2}\delta_{\mathbf{k}_1+q,\mathbf{k}_2}\langle \mathrm{FS}|c^\dagger_{\mathbf{k}_1+q}c_{\mathbf{k}_1+q}c^\dagger_{\mathbf{k}_1}c_{\mathbf{k}_1}|\mathrm{FS}\rangle \\ &= -\delta_{\sigma_1\sigma_2}\delta_{\mathbf{k}_1+q,\mathbf{k}_2}\theta(k_F-|\mathbf{k}_1+q|)\theta(k_F-|\mathbf{k}_1|)\end{aligned} \qquad (4.24)$$

The two delta functions impose the fact that the spin does not change during the interaction and that the momentum is conserved in the process. Furthermore since we can relate $\mathbf{k}_1$ and $\mathbf{k}_2$ we replaced the latter one in the latter operator index.

Here we see the benefit which comes along with this notation. By only using commutation relations for fermion-latter operators we were able to change the rather complicated expression to one that can easily be integrated.

The way to perform this integration can be illustrated graphically Fig.4.2 .

How to choose the boundaries of integration can be illustrated. ...

Second Quantization: Free Electron Gas

$k_F^3 = 3\pi^2 n$

$E_0 = \frac{3}{5}N\epsilon_F$

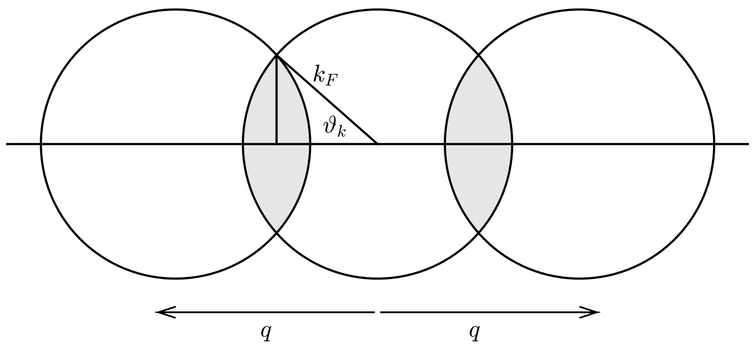

Figure 4.2: illustration of an e-e Interaction were the incoming electrons have initial momentum k_1, k_2 and spin σ_1, σ_2. The interaction V_q causes them to exchange a momentum q.

Bohr Radius: $a_0 = \frac{\hbar}{me^2}$

$$\frac{3\pi^2}{k_F^3} = \frac{1}{n} = \frac{V}{N} = \frac{4\pi}{3}(r_S a_0)^3 \quad \Rightarrow \quad r_S = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{a_0 k_F}$$

$$\frac{E_0}{N} = \frac{2.21}{r_S^2}\frac{e^2}{2a_0}$$

Electron Interaction

$$\frac{E_1}{N} = \frac{\langle FS|\, V_{el-el}\, |FS\rangle}{N} = -\frac{e^2}{2}\frac{V}{N}\frac{k_F^4}{2\pi^3} = -\frac{0.916}{r_S}\frac{e^2}{2a_0}$$

plot - energy minimum at r_S

$$V_{\text{el-el}} = \frac{1}{2V}\sum_{\sigma_1\sigma_2}\sum_{k_1k_2q} V_q c^\dagger_{k_1+q} c^\dagger_{k_2-q} c_{k_2} c_{k_1} \tag{4.25}$$

Chapter 5

Electron-Electron Interaction

5.1 Fermi Liquid Theory

5.2 Electron Tight Binding Model

An approximation for an electron wave function over the whole crystal can be given as

$$\Psi_k = \sum_j c_{kj}\varphi(\mathbf{r}-\mathbf{r}_j) \tag{5.1}$$

Where $\varphi(\mathbf{r})$ is the ground state wave function (atomic orbital) of an electron in the potential $V(\mathbf{r})$ of an isolated atom. This approximation is only valid if the interaction between neighboring atoms is small. The sum goes over all lattice points.

Using

$$c_{kj} = N^{-1/2}e^{i\mathbf{kr}_j} \tag{5.2}$$

The factor $N^{-1/2}$ ensures the wave function to meet the normalization criterion We can express the over all wave function of an electron in the crystal

$$\Psi_k(\mathbf{r}) = N^{-1/2}\sum_j e^{i\mathbf{kr}_j}\varphi(\mathbf{r}-\mathbf{r}_j) \tag{5.3}$$

Recalling the **Bloch Theorem** which states, that the wave function of an electron in a periodic potential ($V(\mathbf{r}) = V(\mathbf{r}+\mathbf{a})$) with the periodicity a is given by

$$\phi_k(\mathbf{r}) \quad = \quad u_k(\mathbf{r}) \cdot e^{i\mathbf{kr}} \tag{5.4}$$

where $u_k(\mathbf{r})$ has the periodicity of the crystal ($u_k(\mathbf{r}+\mathbf{a}) = u_k(\mathbf{r})$). Since the tight binding ansatz is meant to describe the electrons in a periodic potential, so it also have to be a Bloch wave.

We can show, that our electron wave function Eq 5.3 fulfills the Bloch criterion

$$\begin{aligned}
\Psi_k(\mathbf{r}+\mathbf{a}) &= N^{-1/2} \sum_j e^{i\mathbf{kr}_j} \varphi(\mathbf{r}+\mathbf{a}-\mathbf{r}_j) \\
&= N^{-1/2} e^{i\mathbf{ka}} \sum_j e^{i\mathbf{k}(\mathbf{r}_j-\mathbf{a})} \varphi(\mathbf{r}-(\mathbf{r}_j-\mathbf{a})) \\
&= N^{-1/2} e^{i\mathbf{ka}} \sum_n e^{i\mathbf{kr}_n} \varphi(\mathbf{r}-\mathbf{r}_n) \\
&= e^{i\mathbf{ka}} \Psi_k(\mathbf{r})
\end{aligned} \tag{5.5}$$

To get to this result we used the fact, that the summation goes over all lattice points and we therefore can replace the dummy variables j with n by writing $\mathbf{r}_j - \mathbf{a}$ as $\mathbf{r}_n$. This is allowed since $\mathbf{a}$ describes a lattice vector connecting two lattice points.

We can compute now for the energy levels of the tight-binding ansatz

$$\epsilon_k \quad = \quad \langle \mathbf{k}|H|\mathbf{k}\rangle \quad = \quad N^{-1} \sum_j \sum_m e^{i\mathbf{k}(\mathbf{r}_j - \mathbf{r}_m)} \langle \varphi_m|H|\varphi_j\rangle \tag{5.6}$$

The double sum can be understood in the following sense: to get the total energy, we have to sum over all the electrons ($\sum_j$), whereas every electron feels a contribution from the potential of every atom in the crystal ($\sum_m$). Since we assume, that the electrons on an atom site mainly feel interactions on the atom site itself and the nearest neighbors, we can neglect all terms with $j \neq m$ of the first sum. We also define $\rho_m = \mathbf{r}_m - \mathbf{r}_j$

$$\begin{aligned}
\epsilon_k &= \sum_m e^{-i\mathbf{k}\rho_m} \langle \varphi(\mathbf{r}-\rho_m)|H|\varphi(\mathbf{r})\rangle \\
&= \langle \varphi(\mathbf{r})|H|\varphi(\mathbf{r})\rangle \ + \sum_{\rho_m \in \mathrm{NN}} \langle \varphi(\mathbf{r}-\rho_{\mathbf{m}})|H|\varphi(\mathbf{r})\rangle
\end{aligned} \tag{5.7}$$

Defining the coefficients

$$\epsilon_0 \;=\; \langle \varphi(\mathbf{r})|H|\varphi(\mathbf{r})\rangle \;=\; \int d^3\mathbf{r}\; \varphi^*(\mathbf{r})H\varphi(\mathbf{r}) \tag{5.8}$$

$$t \;=\; \langle \varphi(\mathbf{r}-\rho_{\mathbf{m}})|H|\varphi(\mathbf{r})\rangle \;=\; \int d^3\mathbf{r}\; \varphi^*(\mathbf{r}-\rho_{\mathbf{m}})H\varphi(\mathbf{r}) \tag{5.9}$$

allows us to write Eq 5.7 in the abbreviated way

$$\epsilon_k \;=\; \epsilon_0 \;-\; t\sum_{\rho_m} e^{-i\mathbf{k}\rho_m} \tag{5.10}$$

where ϵ_0, the energy level of the single atom, defines the position of the energy band and t, defined through the overlap of neighboring atoms, defines the width of the energy band.

Example: cubic lattice structure

For a cubic lattice structure, taking only the nearest neighbors into account we have to sum over the following lattice sites in the sum of Eq 5.10

$$\rho_m \;\in\; \{(\pm a,0,0),\; (0,\pm a,0),\; (0,0,\pm a)\} \tag{5.11}$$

This leads to the following expression for the energy bands

$$\epsilon_k \;=\; E(\mathbf{k}) \;=\; \epsilon_0 \;+\; 2t\,[\cos(k_x a)+\cos(k_y a)+\cos(k_z a)] \tag{5.12}$$

The position (ϵ_0) and width $W = 12t$ is determined by the particular single atom orbital wave function.

5.3 Charge Ordering

$$\rho(r) \;=\; \rho^{\mathrm{Total}}(\mathbf{r}) \;=\; \rho^{\mathrm{Ext}}(\mathbf{r}) \;+\; \rho^{\mathrm{Ind}}(\mathbf{r}) \tag{5.13}$$

With the Poisson equation we can determine the electric potential ϕ produced by the charge density

$$\nabla^2\phi^{\mathrm{Ext}} \;=\; -\frac{1}{\epsilon_0}\rho^{\mathrm{Ext}}(\mathbf{r}) \tag{5.14}$$

$$\nabla^2\phi \;=\; -\frac{1}{\epsilon_0}\rho(\mathbf{r}) \tag{5.15}$$

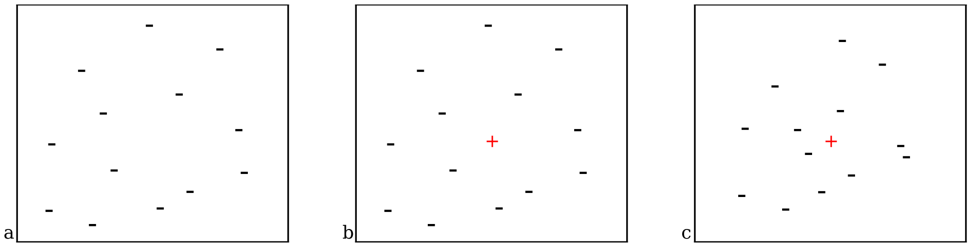

Figure 5.1: Sketch of boxes filled with charged particles. **a.** equally distributed negatively charged particles. **b.** negativel charges with one positive charge without interactions. **c.** negative charged particles are attracted by positive charge.

This differential equation can be solved by transforming it to the Fourier space

$$q^2\phi^{\text{Ext}}(\mathbf{q}) = \frac{1}{\epsilon_0}\rho^{\text{Ext}}(\mathbf{q}) \tag{5.16}$$

$$q^2\phi(\mathbf{q}) = \frac{1}{\epsilon_0}\rho(\mathbf{q}) \tag{5.17}$$

Using the definitions for the dielectric function ϵ and the electric susceptibility χ

$$\frac{1}{\epsilon(\mathbf{q})} = \frac{\phi(\mathbf{q})}{\phi^{\text{Ext}}(\mathbf{q})} \tag{5.18}$$

$$\chi(\mathbf{q}) = \frac{\rho^{\text{Ind}}(\mathbf{q})}{\phi(\mathbf{q})} \tag{5.19}$$

We can relate the dielectric function and the susceptibility by using the formulas for the electric potential from above

$$\epsilon(\mathbf{q}) = 1 - \frac{\chi(\mathbf{q})}{\epsilon_0 q^2} \tag{5.20}$$

5.3.1 Thomas-Fermi Screening

Calculate $\chi(\mathbf{q})$

Charge density of an electron gas can be expressed in terms of the electron density $n(\mathbf{r})$

$$\rho_0 = -en(\mu) \quad \text{with} \quad n(\mu) = \int \frac{d\mathbf{k}}{4\pi^3}\, f_k(\mu) \tag{5.21}$$

The electron density itself is then given as the integral over the Fermi-Dirac distribution. We can write the Schroedinger Equation as

$$-\frac{\hbar^2}{2m}\nabla^2\Psi_k \;-\; e\phi^{\text{Total}}\;\Psi_k \;=\; \varepsilon_k\;\Psi_k \tag{5.22}$$

Using the Thomas-Fermi approximation in which we assume for the total electric potential to be constant on the length scale of our problem. Then we can write

$$\varepsilon_k \;=\; \frac{(\hbar\mathbf{k})^2}{2m} \;+\; \varepsilon' \qquad \text{where} \qquad \varepsilon' \;=\; e\;\phi(\mathbf{r}) \tag{5.23}$$

With this new expression for the electron energy ε_k we are able to write an expression for the electron density $n(\mathbf{r})$ of the whole system

$$\begin{aligned} n^{\text{Total}} \;&=\; \int \frac{d\mathbf{k}}{4\pi^3}\left(e^{(E_k+\mu)/k_BT} \;+\; 1\right)^{-1} \\ &=\; \int \frac{d\mathbf{k}}{4\pi^3}\left(e^{(\frac{(\hbar\mathbf{k})^2}{2m}+\varepsilon'+\mu)/k_BT} \;+\; 1\right)^{-1} \;=\; n(\mu+\varepsilon') \end{aligned} \tag{5.24}$$

As we know from Eq 5.13 the induced charge density is given as the difference between the total charge density $n(\mathbf{r})$ and the external charge density n_0. Therefore we can write

$$\rho^{\text{Ind}}(\mathbf{r}) \;=\; -e\left[n(\mu+\varepsilon') \;-\; n(\mu)\right] \;=\; -e\cdot\varepsilon'\;\frac{dn}{d\mu} \tag{5.25}$$

The difference of the two electron density was replaced by the derivative by using the definition of derivatives $df/dx = (f(x+\Delta x) - f(x))/\Delta x$. Eq 5.25 is known as the basic equation of the Thomas-Fermi Theory. Replacing ε' by the electric potential again and Fourier transforming Eq 5.25 gives

$$\rho^{\text{Ind}}(\mathbf{q}) \;=\; -e^2\frac{dn}{d\mu}\phi(\mathbf{q}) \tag{5.26}$$

Comparing this to Eq 5.19 we found for the susceptibility and the dielectric function

$$\chi \;=\; -e^2\frac{dn}{d\mu} \qquad \text{and} \qquad \epsilon(\mathbf{q}) \;=\; 1+\frac{e^2\;dn/d\mu}{\epsilon_0 q^2} \tag{5.27}$$

It is important to note that the susceptibility does here not depend on the wave vector $\mathbf{q}$. This is a result of our approximation that $\phi(\mathbf{r})$ does not vary much over $\mathbf{r}$.

Thomas-Fermi Wave vector

Defining the Thomas-Fermi wave vector $\mathbf{k}_0 \;=\; \frac{e^2 dn/d\mu}{\epsilon_0}$ allows us to write Eq 5.27 as

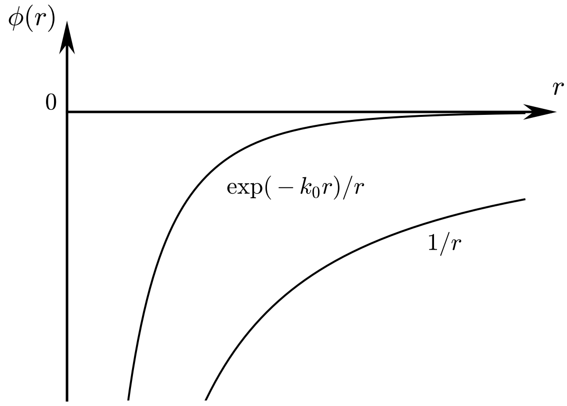

Figure 5.2: Illustration of bare coulomb potential (r^{-1}) and the Yukawa potential.

$$\epsilon(\mathbf{q}) \quad = \quad 1 \; + \; \frac{\mathbf{k}_0^2}{\mathbf{q}^2} \tag{5.28}$$

From this expression it is visible that we can define a characteristic length scale of the electron screening. This length scale is given as $1/\mathbf{k}_0$ and we refer to it as **Thomas-Fermi Screening Length**. For copper we have a screening length of $1/\mathbf{k}_0 = 0.55\,\text{Å}$.

Example: Coulomb Potential

Looking at a point charge Q placed in a sea of conduction electrons, as illustrated in Fig.5.1 .b we can express the external potential generated from the point charge as $\phi^{\text{Ext}}(\mathbf{r}) = Q/r$ with its Fourier transform $\phi^{\text{Ext}}(\mathbf{q}) = 4\pi Q/q^2$. Rearranging Eq **??** and replacing the dielectric function by Eq 5.28 , we obtain

$$\phi(\mathbf{q}) \quad = \quad \frac{\phi^{\text{Ext}}(\mathbf{q})}{\epsilon(\mathbf{q})} \quad = \quad \frac{4\pi \; Q}{q^2 + k_0^2} \tag{5.29}$$

Fourier transform this back to real space leads to the well known **Yukawa Potential**

$$\phi(\mathbf{r}) \quad = \quad Q\frac{e^{-k_0 r}}{r} \tag{5.30}$$

The difference between the Coulomb- and Yukawa potential are displayed in Fig.5.2 . The screening effect added point charge by the surrounding negative charges is clearly visible in the faster convergence to zero of the Yukawa Potential. The screening also weakens the long range interaction of the charges in the solid.

5.3.2 Lindhard Potential

A more sophisticated approach is provided by the Lindhard Theory from which the Thomas-Fermi screening is a special case ($\mathbf{q} \ll \mathbf{k}_0$). The basic idea here is to find a solution for the Schroedinger equation by treating the electrical potential $\phi^{\text{Ext}}(\mathbf{r})$ introduced by the external charge as a perturbation, which allows us then to use the methodology of perturbation theory.

As we know, the charge density for one electron with momentum $\mathbf{k}$ is given as $\rho_{\mathbf{1}}(\mathbf{r}) = e|\psi_{\mathbf{k}}(\mathbf{r})|^2$. Describing the the overall charge density of a crystal, assuming it is in its ground state we have to sum the one electron charge density multiplied with the Fermi function $f_{\mathbf{k}}$ over all momenta $\mathbf{k}$

$$\rho(\mathbf{r}) \quad = \quad -e\sum_{\mathbf{k}} f_{\mathbf{k}}|\Psi_{\mathbf{k}}(\mathbf{r})|^2 \tag{5.31}$$

As mentioned above, assuming the term $e\phi$ as perturbation, we can express the electron wave vector $\psi_{\mathbf{k}}$ as

$$\psi_{\mathbf{k}} \quad = \quad |\mathbf{k}_0\rangle \ + \ {\sum_{\mathbf{k}}}' \frac{\langle\mathbf{k}'|e\phi|\mathbf{k}_0\rangle}{\varepsilon_{\mathbf{k}_0} - \varepsilon_{\mathbf{k}'}} \ |\mathbf{k}'\rangle \tag{5.32}$$

To plug our ansatz for $\psi_{\mathbf{k}}$ into Eq 5.31 we evaluate first

$$\begin{aligned} |\psi_{\mathbf{k}}|^2 \quad &= \quad \left(|\mathbf{k}_0\rangle \ + \ \sum_{\mathbf{k}'} \ ... \ |\mathbf{k}'\rangle\right)\left(\langle\mathbf{k}_0| \ + \ \sum_{\mathbf{k}'} \ ... \ \langle\mathbf{k}'|\right) \\ &= \quad \langle\mathbf{k}_0|\mathbf{k}_0\rangle \ + \ \underbrace{\sum_{\mathbf{k}'} \ ... \ \langle\mathbf{k}_0|\mathbf{k}'\rangle}_{A} \ + \ \underbrace{\sum_{\mathbf{k}'} \ ... \ \langle\mathbf{k}_0|\mathbf{k}'\rangle}_{B} \ + \mathcal{O}(2) \end{aligned} \tag{5.33}$$

Using this equation we can write the charge density Eq 5.31 in the following way

$$\rho^{\text{Ind}}(\mathbf{r}) \quad = \quad -e\sum_{\mathbf{k}} \left(|\Psi_{\mathbf{k}}|^2 \ - \ 1\right) \quad = \quad -e\sum_{\mathbf{k}} f_{\mathbf{k}}(A+B) \tag{5.34}$$

Simplifying this equation is easier in Fourier space

$$\rho^{\text{Ind}}(\mathbf{q}) \quad = \quad \int \rho^{\text{Ind}}(\mathbf{r}) \ e^{i\mathbf{q}\mathbf{r}} d^3\mathbf{r} \quad = \quad -e\int d^3\mathbf{r} \ \sum_{\mathbf{k}} f_{\mathbf{k}} \ (A+B) \cdot e^{i\mathbf{q}\mathbf{r}} \tag{5.35}$$

Calculating the Fourier transform for the two variables A and B works similar. We set $\mathbf{k}' = \mathbf{k} + \mathbf{q}$. This gives

$$-e\int d^3\mathbf{r}\ \sum_{\mathbf{k}} f_{\mathbf{k}}\ A\cdot e^{i\mathbf{qr}} \quad = \quad -e\int d^3\mathbf{r}\sum_{\mathbf{k}'}\sum_{\mathbf{k}} f_{\mathbf{k}} \frac{\overbrace{\langle \mathbf{k}-\mathbf{q}|e\phi(\mathbf{r})|\mathbf{k}\rangle}^{\text{FT of }\phi(\mathbf{r})}}{\varepsilon_{\mathbf{k}}\ -\ \varepsilon_{\mathbf{k}-\mathbf{q}}}$$

$$= \quad -e^2\sum_{\mathbf{k}'}\sum_{\mathbf{k}} \frac{f_{\mathbf{k}}\ \phi(\mathbf{q})}{\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{q}}} \tag{5.36}$$

The same goes for the variable B

$$-\ e\int d^3\mathbf{r}\ \sum_{\mathbf{k}'} f_{\mathbf{k}}\ B\cdot e^{i\mathbf{qr}} \quad = \quad -e^2\sum_{\mathbf{k}'}\sum_{\mathbf{k}} \frac{f_{\mathbf{k}'+\mathbf{q}}\ \phi(\mathbf{q})}{\varepsilon_{\mathbf{k}'+\mathbf{q}}-\varepsilon_{\mathbf{k}'}} \tag{5.37}$$

With these expressions for A and B and the definition of the electric susceptibility $\chi(\mathbf{q})$ (Eq 5.19) we can write

$$\chi(\mathbf{q}) \quad \propto \quad \int \frac{d^2\mathbf{k}}{(2\pi)^n}\ \frac{f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}}}{\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{q}}} \qquad \text{with the dimensionality } n\in\{1,2,3\} \tag{5.38}$$

By knowing the band structure one can now calculate $\chi(\mathbf{q})$. In this way one is able to experimentally measure the screening potential.

picture Lindhard susceptibility for different dimensions

Chapter 6

Magnetism

6.1 Paramagnetism

Magnetic Moment

insert picture - magnetic moment

If $\vec{A}$ is the area inside the loop and I the current, the magnetic moment can be written as

$$\vec{\mu} = I\vec{A} \tag{6.1}$$

Example: Hydrogen Atom

insert picture - hydrogen atom and orbiting electron

The magnetic moment of a hydrogen atom can be described semi-classically by assuming the electron to be on a fixed trajectory orbiting the hydrogen nucleus with constant radius r and velocity v. The current I produced by the moving electron can be written as $I = -e/\tau$ with the orbital period $\tau = 2\pi r/v$. For the loop area we use the formula $A = \pi r^2$. This leads to the magnetic moment

$$\mu = \frac{-ev\pi r^2}{2\pi r} = \frac{-evr}{2} = \frac{-emvr}{2m} \tag{6.2}$$

We can identify the classical definition of the angular momentum $\vec{l} = \vec{r} \times m\vec{v}$ in the numerator. Taking the quantization of angular momentum $|\hat{l}| = n\hbar$ in quantum mechanics into account we can rewrite expression 6.2 for $n = 1$

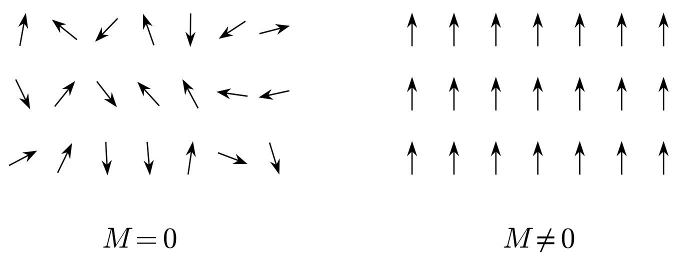

Figure 6.1: hohohoh

$$\mu \;=\; \frac{-e\hbar}{2m} \;\equiv\; -\mu_B \tag{6.3}$$

Which we define as the Bohr magneton μ_B.

Magnetic Moment of Atoms

The total angular momentum in an atom is given as the sum of total orbital angular Momentum $\hat{L}$ and total spin angular momentum $\hat{S}$

$$\hat{J} \;=\; \hat{L} \;+\; \hat{S} \tag{6.4}$$

Magnetization

Considering a solid with N atoms each having a magnetic moment $\vec{\mu}$. We define the magnetization as

$$\vec{M} \;\equiv\; \frac{\text{Sum over all magnetic moments}}{\text{Volume}} \tag{6.5}$$

Magnetic Moment in a $\vec{B}$-Field

From classical electrodynamics we know that the potential energy E of a magnetic moment $\vec{\mu}$ in a magnetic field $\vec{B}$ is described as

$$E \;=\; -\vec{\mu} \,\cdot\, \vec{B} \tag{6.6}$$

To get a feeling for the order of magnitudes of magnetic energy of atomic scale we look at the following example

$$\mu_B \times 1\text{Tesla} \simeq 0.05\,\text{meV}$$

This is comparable to the energy one has to put into a system to increase its temperature by 1 K ($k_B \cdot 1\,\text{K} \simeq 0.084\,\text{meV}$).

Magnetic susceptibility

$$\chi \simeq \frac{\mu_0 \vec{M}}{\vec{B}} \tag{6.7}$$

We can look at the magnetic susceptibility χ as response function. χ describes the response of the system $\vec{M}$ when exposed to an external changing field $\vec{B}$. To simplify things in the calculations we will make the following constraints on $\vec{B}$.

$$\begin{aligned} \vec{B} \text{ is static} \quad &\Rightarrow \quad \text{no time dependence} \\ \vec{B} \text{ is homogeneous} \quad &\Rightarrow \quad \text{no depencence on } \vec{r} \end{aligned}$$

The definition of the susceptibility allows us now to classify materials depending on how they respond to an external magnetic field. We call materials to be *paramagnetic* if they align their spin parallel to the applied $\vec{B}$-Field. This is the case if $\chi > 0$. On the contrary we refer to materials as *diamagnetic* if their inner magnetic moments align anti-parallel with respect to an applied field $\vec{B}$. This results in a negative value for the susceptibility $\chi < 0$.

In reality, the response of systems is composed of multiple different responses which can have different origins.

$$\chi_{total} \simeq \chi_{\text{paramagnetic}} + \chi_{\text{diamagnetic}} + \cdots \tag{6.8}$$

Paramagnetism and diamagnetism can also have different origins. For example:

$$\begin{aligned} \chi_{\text{paramagnetic}} &\simeq \chi_{\text{Langevin}} + \chi_{\text{Van Vleck}} + \chi_{\text{Pauli}} + \cdots. \\ \chi_{\text{diamagnetic}} &\simeq \chi_{\text{electronic}} + \chi_{\text{superconductivity}} + \cdots \end{aligned}$$

Diamagnetism

insert picture - loop current to illustrate lens law

To symbolize diamagnetic behavior we recall lenz's law. It states, that a changing magnetic field induces a current which creates a magnetic field that points in the opposite direction as the initial magnetic field change. In that way the system tries to compensate the externally induced field changes.

To describe that, we use 6.1, with the area $\vec{A} = \pi < r^2 >$ and the current $I = -Ze/\tau$ with the number of electrons Z per atom and the orbit period τ. Expressing the orbit period in terms of the *cyclotron frequency* $\omega = eB/2m$ shows the dependency on the magnetic field.

$$\tau = \frac{2\pi}{\omega} = \frac{4\pi m}{eB} \tag{6.9}$$

Putting everything together we get the following expression to approximate the magnetic moment of a diamagnet

$$\vec{\mu} = -\frac{Ze^2 B}{4\pi m}\pi < r^2 > = -\frac{Ze^2 B}{4m} < r^2 > \tag{6.10}$$

The magnetization of a macroscopic material can be written as the sum over all the magnetic moments of its atoms resulting in

$$\vec{M} = \mu_0 N \vec{\mu} \tag{6.11}$$

where N denotes the number of atoms per volume. Recalling 6.7, we find for the diamagnetic susceptibility caused by electrons

compare formula with wikipedia. probably wrong by a prefactor

$$\chi_{\text{Diamagnetic}} = -\frac{\mu_0 N Z e^2}{4m} < r^2 > \tag{6.12}$$

Simplest Case: e^- only

Consider a system consisting of atoms with only one electron

$$\rightarrow \quad \hat{L} = 0, \quad \hat{S} \simeq 1/2 \qquad \Rightarrow \quad \hat{J} = 1/2 \tag{6.13}$$

Furthermore we assume for the spin g-factor $g \simeq 2$ (not proved). This system has only two states: *spin-up* and *spin-down*. The Energy of this states in an external magnetic field is given by

$$E = -\vec{\mu} \cdot \vec{B} = \pm \mu_B \cdot |\vec{B}| \tag{6.14}$$

vector diagram energy consideration of magnetic moment in B-field

As stated before, the Energy resulting from magnetic moments of the order of magnitude of a Bohr magneton μ_B to magnetic fields to several Tesla are in the same energy range of some Kelvin (some $k_B T$). Therefore we use Boltzmann statistics to describe the **population distribution** of the system. The probability of energy level E_1 to be populated can be written as

$$p_\alpha = \frac{e^{\beta E_\alpha}}{\mathcal{Z}} = \frac{e^{\beta E_\alpha}}{e^{\beta E_1} + e^{\beta E_2}}, \quad \text{with} \quad \alpha = \{1, 2\} \tag{6.15}$$

where $\beta = 1/k_B T$ and the partition function $\mathcal{Z} = \sum_i e^{\beta E_i}$.

$$p_1 = \frac{e^{\beta E_1}}{e^{\beta E_1} + e^{-\beta E_1}}, \quad p_2 = \frac{e^{-\beta E_1}}{e^{\beta E_1} + e^{-\beta E_1}} \tag{6.16}$$

This has to be equal to $p_1 = N_1/N$ and $p_2 = N_2/N$ with N_1 (N_2) being the number of electrons in the energy state E_1 (E_2) and $N = N_1 + N_2$ being the total number of electrons in the system. Furthermore we substitute $\bar{x} = \beta E_1 = \mu_B B/k_B T$.

plots energy level population

The magnetization M can now be written as the difference in the number of electrons with opposite magnetic moment

$$\begin{aligned} M &= (N_1 - N_2)\mu_B = N\mu_B(\frac{N_1}{N} - \frac{N_2}{N}) = N\mu_B \left(\frac{e^{\bar{x}} - e^{-\bar{x}}}{e^{\bar{x}} + e^{-\bar{x}}}\right) \\ M &= N\mu_B \tanh(\bar{x}) \end{aligned} \tag{6.17}$$

Looking at the case $\bar{x} \ll 1$, which stands for having large temperatures and/or low magnetic fields. We get for the magnetization

$$M \simeq N\mu_B \bar{x} = N\frac{\mu_B^2 B}{k_B T} \tag{6.18}$$

With the help of this equation we can now write down an expression for the paramagnetic susceptibility for (large temperature or low magnetic fields)

$$\chi_{\text{paramagnet}} = \frac{N\mu_B^2}{k_B T} \tag{6.19}$$

We refer to this formula as *Curie law* and we call the introduced constant $C = N\mu_B^2/k_B$ *Curie-constant.*

6.1.1 How to fill the valence shell

Hund's rules

The Hund's rules provide simply rules which give an idea about the total spin-, total orbital- and total angular momentum of an atom in its ground state

1. Maximize S to minimize the Coulomb energy
2. Maximize L to minimize Coulomb repulsion
3. $J = |L - S|$ for less than half filling and $J = |L + S|$ for more than half filling.

Crystal field effects

Atoms arranged in a lattice feel the presence of the atoms around. This happens in a way, that the valence electrons of the atom under consideration are experiencing the electric field from the ligands surrounding the atom. That causes the energy degeneracy, apparent in a free atom, to be lifted. This splitting of energy levels has impact on the occupation of the different orbitals when "filling" the atom with electrons. For studying this effect now we will consider the valence electrons to partially fill the $3d$-orbital because this is also the case in a variety of materials in nature. Partially filled $3d$-bands can especially be found in the *Transition metals*. We now exemplify that at at systems with ligands arranged octahedral and tetragonal.

Octahedral crystal environment

Tetrahedral crystal environment

Variation of crystal field environment

Jahn-Teller Distortion

complete this subsubsection with infos from lecture notes

Resonant inelastic x-ray scattering (RIXS)

6.2 Ferromagnetism

6.2.1 H_2 Molecule

Wave Function Considerations

$$\begin{aligned} \Psi^{Total}(2 \text{ Electrons}) &\rightarrow \text{Antisymmetric} && (6.20) \\ \Psi^{Total}(\vec{r}_1, \vec{r}_2) &= -\Psi^{Total}(\vec{r}_2, \vec{r}_1) && (6.21) \end{aligned}$$

$$\begin{aligned} \Psi_A &= \psi_\alpha(\vec{r}_1)\psi_\beta(\vec{r}_2) - \psi_\alpha(\vec{r}_2)\psi_\beta(\vec{r}_1) && (6.22) \\ \Psi_S &= \psi_\alpha(\vec{r}_1)\psi_\beta(\vec{r}_2) + \psi_\alpha(\vec{r}_2)\psi_\beta(\vec{r}_1) && (6.23) \end{aligned}$$

Consider now spin wave function:

$$\chi_S = \chi_{Symmetric} = \begin{cases} |\uparrow_\alpha\uparrow_\beta\rangle & = |1,1\rangle \\ (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2} & = |1,0\rangle \\ |\downarrow_\alpha\downarrow_\beta\rangle & = |1,-1\rangle \end{cases} \quad (6.24)$$

$$\chi_A = \chi_{Antisymmetric} = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2} \quad |0,0\rangle \quad (6.25)$$

Where to the χ_S is referred to as **Triplet state** and to the wave function χ_A is referred to as **singlet state**.

Quantum mechanical Spin-Operators

Recalling that $\hat{S}^2|S,m\rangle = S(S+1)|S,m\rangle$ we get for the eigenvalues of $\hat{S}_\alpha^2$ and $\hat{S}_\beta^2$

$$\begin{aligned} \hat{S}_\alpha^2|S_\alpha,m\rangle &= S_\alpha(S_\alpha+1)|S_\alpha,m\rangle &= 3/4 && (6.26) \\ \hat{S}_\beta^2|S_\beta,m\rangle &= S_\beta(S_\beta+1)|S_\beta,m\rangle &= 3/4 && (6.27) \end{aligned}$$

$$\hat{S} = \hat{S}_\alpha + \hat{S}_\beta \Rightarrow \hat{S}^2 = \hat{S}_\alpha^2 + \hat{S}_\beta^2 + 2\hat{S}_\alpha\hat{S}_\beta \Rightarrow \hat{S}_\alpha \cdot \hat{S}_\beta = \frac{\hat{S}^2 - \hat{S}_\alpha^2 - \hat{S}_\beta^2}{2} \quad (6.28)$$

Calculating $\langle\hat{S}_\alpha \cdot \hat{S}_\beta\rangle$ leads to $1/4$ for χ_S and $-3/4$ for the χ_A case.

Consider weak Coulomb interaction

$$H \quad = \quad H_{\text{single-H}} \; + \; H_{\text{int}} \quad = \quad H_0 \; + \; H_{\text{int}} \tag{6.29}$$

Where the interaction Hamiltonian H_{int} includes the proton-proton, electron-electron, proton 1 - electron 2 and electron 1 - proton 2 interactions.

$$H_{int} \quad = \quad \frac{e^2}{d_{pp}} \; + \; \frac{e^2}{d_{ee}} \; - \; \frac{e^2}{d_{ep}} \; - \; \frac{e^2}{d_{pe}} \tag{6.30}$$

Here d_{pp} stands for the proton-proton distance, d_{ee} for the electron-electron distance. Furthermore contains $H_{\text{single-H}}$ both Hamiltonians of the single hydrogen atoms

$$H_{\text{single-H}} \quad = \quad H_{H_1} \; + \; H_{H_2} \quad = \quad \frac{\hbar}{2m}\left(\nabla_\alpha^2 + \nabla_\beta^2\right) \; - \; \left(\frac{e^2}{d_{p_\alpha e_\alpha}} + \frac{e^2}{d_{p_\beta e_\beta}}\right) \tag{6.31}$$

$$E_+ \; = \; E_S \quad = \quad \langle \Psi_S | H_{\text{int}} | \Psi_S \rangle \quad = \quad \int (\psi_\alpha\, \psi_\beta + \psi_\beta\, \psi_\alpha)^* H_{\text{int}} (\psi_\alpha\, \psi_\beta + \psi_\beta\, \psi_\alpha) d^3r \tag{6.32}$$

$$E_- \; = \; E_A \quad = \quad \langle \Psi_A | H_{\text{int}} | \Psi_A \rangle \quad = \quad \int (\psi_\alpha\, \psi_\beta - \psi_\beta\, \psi_\alpha)^* H_{\text{int}} (\psi_\alpha\, \psi_\beta - \psi_\beta\, \psi_\alpha) d^3r \tag{6.33}$$

Introducing the terms J_1, J_2, C_1 and C_2 indicated in Eq 6.32 and Eq 6.33

$$J_1 \;\equiv\; \int \psi_\alpha^* \psi_\beta^* H_{\text{int}} \psi_\beta \psi_\alpha d^3r \; , \qquad J_2 \;\equiv\; \int \psi_\beta^* \psi_\alpha^* H_{\text{int}} \psi_\alpha \psi_\beta d^3r \tag{6.34}$$

$$C_1 \;\equiv\; \int \psi_\alpha^* \psi_\beta^* H_{\text{int}} \psi_\alpha \psi_\beta d^3r \; , \qquad C_2 \;\equiv\; \int \psi_\beta^* \psi_\alpha^* H_{\text{int}} \psi_\beta \psi_\alpha d^3r \tag{6.35}$$

By further defining $C \equiv C_1 + C_2$ and $J \equiv J_1 + J_2$ one can write the two energies as

$$E_\pm \quad = \quad C \; \pm \; J \tag{6.36}$$

Furthermore for the difference of the singlet- and triplet energy we get

$$E_+ - E_- \quad = \quad 2J \quad = \quad 4 \int \psi_\alpha^* \psi_\beta^* H_{\text{int}} \psi_\beta \psi_\alpha d^3r \tag{6.37}$$

From this equation we can associate the introduced variable J as the **Exchange Integral**.

$$J \quad = \quad \frac{E_+ - E_-}{2} \quad = \quad 2 \int \psi_\alpha^* \psi_\beta^* H_{\text{int}} \psi_\beta \psi_\alpha d^3r \tag{6.38}$$

What is $\mathbf{H^{Spin}}_{\mathbf{int}}$

$$E_{\pm} \;=\; C \pm J \;=\; C - J/2 - 2J \cdot \langle \hat{S}_{\alpha} \cdot \hat{S}_{\beta} \rangle \;=\; \text{constant} + 2J\langle \hat{S}_{\alpha} \cdot \hat{S}_{\beta} \rangle \quad (6.39)$$

The constant contribution to the energies $E_{\pm}$ can be neglected since absolute energies values are arbitrary. The interesting term for us is the second one on the right-most side. It gives us a quantitative measure of how large the energy difference between the two spin configurations is

$$\Rightarrow \quad H_{\text{int}}^{\text{Spin}} \;=\; -2J\hat{S}_{\alpha} \cdot \hat{S}_{\beta} \qquad \begin{cases} J > 0 & \Rightarrow \quad E_S > E_A \quad \Rightarrow \quad \chi_S \text{ favorable} \\ J < 0 & \Rightarrow \quad E_A < E_S \quad \Rightarrow \quad \chi_A \text{ favorable} \end{cases} \quad (6.40)$$

From the upper formula we see that J tells if χ_S or χ_A is preferred because it determines which energy (E_S or E_A) is lower. Therefore J can be seen as an indication if ferro- or antiferromagnetism is present in a material.

Ferromagnetism

$$\begin{aligned} H &= -\sum_{ij} J_{ij}\vec{S}_i \cdot \vec{S}_j + g\mu_B \cdot \sum_j \vec{S}_j \cdot \vec{B} \\ &= -\sum_j \sum_i J_{ij}\vec{S}_i \cdot \vec{S}_j + g\mu_B \sum_j \vec{S}_j \cdot \vec{B} \\ &= g\mu_B \sum_j \vec{S}_j \cdot (\underbrace{\vec{B}_{mf}}_{\text{internal}} + \underbrace{\vec{B}}_{\text{external}}) \end{aligned} \quad (6.41)$$

Using a mean field approximation we rewrite the interaction from all spins on $\vec{S}_j$ from the first term as with a mean magnetic field $\vec{B}_{mf}$ whereas we define $\vec{B}_{mf} \equiv -2/g\mu_B \sum_i J_{ij}\vec{S}_i$.

Conjecture

By making an educated guess one could assume, that the mean magnetic field $\vec{B}_{mf}$ can be approximated macroscopically with the following expression.

$$\vec{B}_{mf} \;\simeq\; \lambda \cdot \vec{M} \quad (6.42)$$

Solution

Solution can be adapted from the results about paramagnetism we gained last week. By focusing on the case $\vec{B} = 0$ we get

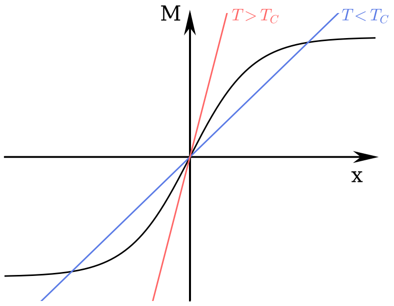

Figure 6.2: Illustration of the grafical solution of 6.43. the straight lines refer to different values of T.

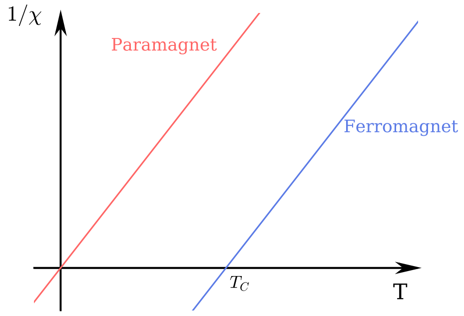

Figure 6.3: Illustration of inverse susceptibility χ of a Para- and Ferromagnet.

$$M \simeq N\mu_B \tanh(x) \quad \text{with} \quad x = \frac{\mu_B}{k_B T}(\vec{B} + \lambda\vec{M}) \tag{6.43}$$

Since the argument of the hyperbolic tangent depends also on the magnetization $\vec{M}$ we have an implicit equation. A solution of this equation is illustrated in Fig.6.2 as the crossing point between the hyperbolic tangent and the straight line. In this graph it is also visible, that above a certain Temperature $T > T_C$ there only exists one solution for the implicit equation which can be associated with the paramagnetic phase of the material. On the other hand for $T < T_C$ we see that there are exists multiple solution of 6.43 which is in accordance with the magnetization curve of a ferromagnet. We can determine the Transition temperature T_C by comparing the slopes of the two curves at the origin

$$\frac{d}{dx} N\mu_B \tanh(x)\bigg|_{x=0} = \frac{d}{dx}\frac{k_B T}{\mu_B \lambda} x \quad \Rightarrow \quad T_C = \frac{\lambda N \mu_B^2}{k_B} = \lambda \cdot C \tag{6.44}$$

Looking at the limit $x \ll 1$

$$\left.\begin{array}{lll} M & = & CB/T \\ \chi & \equiv & M/B = C/T \end{array}\right\} \rightarrow \begin{array}{lll} M & = & C\frac{B+\lambda M}{T} \\ \chi & \equiv & \frac{C}{T} + \frac{\lambda C}{T}\chi \end{array} \Rightarrow \chi = \frac{C}{T - \lambda C} = \frac{C}{T - T_C}$$

Checking the magnetization $M(T)$ at zero field $\vec{B} = 0$. Using 6.43 with zero field and the definitions $m = M/N\mu_B$ and $t = k_B T/N\mu_B^2\lambda = T/T_C$ we get

$$m = \tanh\left(\frac{m}{t}\right) \tag{6.45}$$

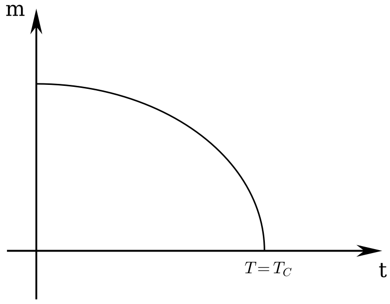

Figure 6.4: Temperature dependence of magnetisation.

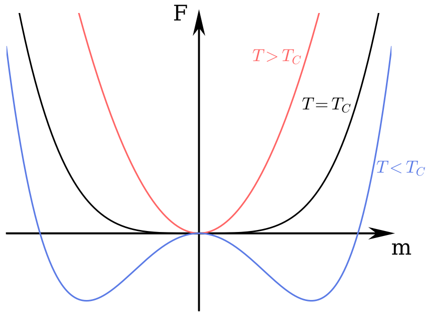

Figure 6.5: Free Energy dependence on the order parameter m for the 3 cases $T < T_C$, $T = T_C$ and $T > T_C$.

Landau Theory

According to the Landau theory of phase transition the free energy F can be expressed

$$F = F_0 + a(T)m^2 + bm^4 + \ldots \tag{6.46}$$

Were the parameter a and b has to meet the conditions

$$a(T) = a_0(T - T_C) \quad \text{and} \quad b > 0 \tag{6.47}$$

We find the thermodynamical state of our system by minimizing the free energy

$$\frac{dF}{dm} = m(2a(T) + 4bm^2) = 0 \quad \Rightarrow \quad m = \begin{cases} 0 \\ \pm\sqrt{\frac{a_0(T-T_C)}{2b}} \end{cases} \tag{6.48}$$

6.2.2 Exchange Interaction J

Analog to the susceptibility of ferromagnets $\chi_{FM} = C/(T - T_C)$, we can define the susceptibility for antiferromagnets

$$\chi_{AFM} = \frac{C}{T + T_N} \tag{6.49}$$

Where we refer to the Transition Temperature T_N as Neel-Temperature.

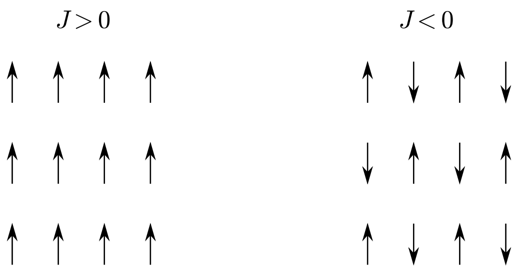

Figure 6.6: hohoho

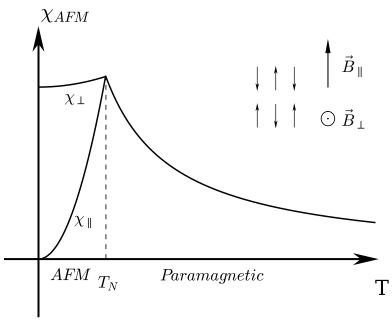

Figure 6.7: Temperature dependence of magnetisation.

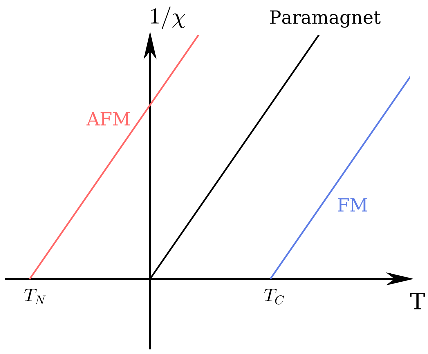

Figure 6.8: Free Energy dependence on the order parameter m for the 3 cases $T < T_C$, $T = T_C$ and $T > T_C$.

6.2.3 Ferromagnetic Magnons

Consider a linear FM chain $|\text{FM}\rangle = |\uparrow\uparrow\uparrow \,...\,\rangle$. Applying the latter operator s_j^- on $|\text{FM}\rangle$ leads to

$$|j\rangle = s_j^-|\text{FM}\rangle = |\uparrow\uparrow \,...\, \uparrow \underbrace{\downarrow}_{j} \uparrow \,...\,\rangle \tag{6.50}$$

Defining

$$|q\rangle = \frac{1}{\sqrt{N}}\sum_j e^{iqR_j}|j\rangle \tag{6.51}$$

The Hamiltonian is given by

$$
\begin{aligned}
H &= -\sum_{ij} J_{ij}\hat{S}_i \cdot \hat{S}_j \quad = \quad -2J\sum_i \hat{S}_i \cdot \hat{S}_{i+1} \\
&= -2J\sum_i \left\{ \hat{S}_i^z \hat{S}_{i+1}^z \; + \; \frac{1}{2}\left[\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+\right]\right\} \qquad (6.52)
\end{aligned}
$$

The second equality sign holds if we only take nearest neighbor interactions into account. To get the final expression we used the substitution

$$
\hat{S}^2 \quad = \quad \hat{S}^{z^2} \; + \; \frac{1}{2}\left[\hat{S}^+\hat{S}^- + \hat{S}^-\hat{S}^+\right] \qquad (6.53)
$$

$$
H|\mathrm{FM}\rangle \quad = \quad -2JNS^2|\mathrm{FM}\rangle \quad = \quad E_0|\mathrm{FM}\rangle \qquad (6.54)
$$

$$
H|j\rangle \quad = \quad -2J\left\{(N-4)S^2|j\rangle \; + \; S\left[|j+1\rangle + |j-1\rangle\right]\right\} \qquad (6.55)
$$

$$
\begin{aligned}
H|q\rangle &= \frac{1}{\sqrt{N}}\sum_j e^{iqR_j}\left\{NS^2|j\rangle \; - \; 2S^2|j\rangle \; + \; S|j+1\rangle \; + \; S|j-1\rangle\right\} \\
&= -2JNS^2|q\rangle - 2J\left\{-2S^2 \; + \; \left(e^{iqa} + e^{-iqa}\right)\right\}|q\rangle \\
&= E_0|q\rangle \; + \; 2JS\left\{1 - \cos(qa)\right\}|q\rangle \qquad (6.56)
\end{aligned}
$$

Since we are considering an infinite long one dimensional chain of spin states we can rewrite the expression

$$
H|q\rangle \quad = \quad E_0|q\rangle + 2JS\left\{2 - 2\cos(qa)\right\}|q\rangle \qquad (6.57)
$$

which leads to

$$
H|q\rangle \quad = \quad E(q)|q\rangle \qquad \text{with} \qquad E(q) \;\simeq\; E_0 + 2JS(2 - 2\cos(qa)) \qquad (6.58)
$$

This is the dispersion relation for ferromagnets. For antiferromagnets we have a similar relation (not derived)

$$
\hbar\omega \quad = \quad 2J|\sin(qa)| \qquad (6.59)
$$

add qualitative discussion about dispersion relation. mention differences between FM and AFM. Similarities between AFM and phonons.

Chapter 7

Superconductivity

7.1 Conventional superconducters

7.1.1 Link ρ & Meissner Effect

As we know, superconductors are characterized by vanishing resistivity ($\rho = 0$) for undergoing a critical temperature T_C (Fig.7.1). Recalling Ohm's law,

$$\vec{j} = \sigma \vec{E} \tag{7.1}$$

which relates the electron current density $\vec{j}$ and the electric field inside a conductor $\vec{E}$ by introduction the material dependent conductivity σ.

Looking at the case of superconductors, we can emphasize, by rearranging Ohm's law, that the electric field vanishes.

$$\vec{E} = \frac{1}{\sigma}\vec{j} = \rho\vec{j} \simeq 0 \tag{7.2}$$

By using one of the Maxwell equation $\nabla \times \vec{E} = -d\vec{B}/dt$ we can conclude, that for a vanishing electric field $\vec{E} = 0$ there can't be a change of the magnetic field over time $d\vec{B}/dt = 0$.

diagram vanishing B-field

7.2 London Equation

The Lonodon equation is a macroscopic theory that was one of the first theories which allowed to describe effects like the Meissner-Ochsenfeld effect quantitatively. We now want

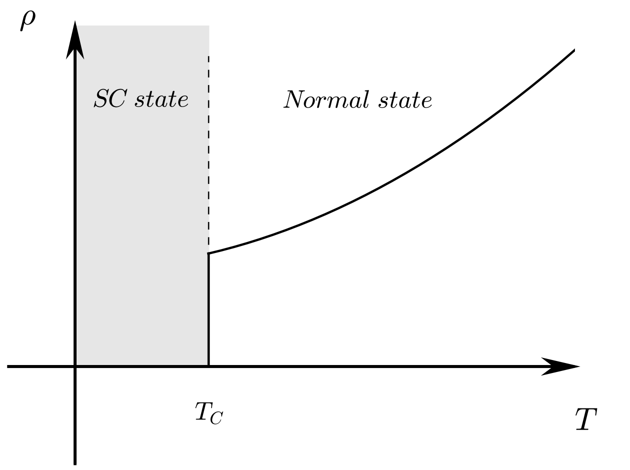

Figure 7.1: hohoho

to qualitatively derive the London equation. For that consider a current oscillating if the frequency ω

$$\vec{j}e^{-i\omega t} = \sigma(\omega)\vec{E}e^{-i\omega t} \tag{7.3}$$

Using the expression for the conductivity $\sigma(\omega)$ from the Drude model for a time-dependent electric field

$$\sigma(\omega) = \frac{\vec{j}}{\vec{E}} = \frac{ne^2\tau}{m}\frac{1}{1-i\omega\tau} \tag{7.4}$$

From this we get, as already proven in a previous exercise, that the real part of the conductivity can be written in the limit of $\tau \to \infty$ as

$$\mathrm{Re}(\sigma(\omega)) = \frac{\pi ne^2}{m}\delta(\omega) \tag{7.5}$$

This can also be made clear, when looking at the limits

$$\mathrm{Re}(\sigma(\omega)) = \frac{ne^2}{m}\frac{\tau}{1+\omega\tau} \xrightarrow{\omega\to 0} \frac{ne^2\tau}{m} \tag{7.6}$$

$$\sigma(\omega) \xrightarrow{\tau\to\infty} -\frac{ne^2}{im\omega} = \mathrm{Im}(\sigma(\omega)) \quad \Rightarrow \quad \mathrm{Re}(\sigma(\omega)) = 0 \qquad \text{for } \omega \neq 0 \tag{7.7}$$

From Eq.7.5 , we see that in the regime of very large mean free times τ between ionic collisions, the real part of the conductivity $\sigma(\omega)$ is only different from zero for vanishing oscillations of the electric field.

To derive the London equation, the following two assumptions have to be made

1. $\tau \to \infty$, which is given since there are no collisions between electrons and lattice ions in the superconducting state.
2. We have to split up the conductivity in a part $\sigma_N(\omega)$ of normal state electrons and a conductivity contribution due to *super electrons* σ_S: $\sigma(\omega) = \sigma_N(\omega) + \sigma_S(\omega)$, were only $\sigma_S(\omega) \neq 0$ in the superconducting state

Taking the curl of the oscillating current

$$\begin{aligned} \nabla \times (\vec{j}e^{-i\omega t}) &= \sigma(\omega)\nabla \times (\vec{E} \cdot e^{-i\omega t}) = -\sigma(\omega)\frac{d}{dt}(\vec{B} \cdot e^{-i\omega t}) \\ &= -\frac{n_S e^2}{m}\vec{B} \cdot e^{-i\omega t} \end{aligned} \tag{7.8}$$

Here we used Eq.7.3 in the first and Farraday's law ($\nabla \times \vec{E} = -d/dt\vec{B}$) in the second step. Furthermore is only the *super electron* density n_S contributing to the conductivity $\sigma(\omega)$. From this equation we can deduce that

$$\nabla \times \vec{j} \propto \vec{B} \qquad \text{and thereof} \quad \vec{j} = -\frac{n_S e^2}{m}\vec{A} \tag{7.9}$$

with $\vec{A}$ being the vector potential. The equation describing this proportionality between the current density $\vec{j}$ and the vector potential $\vec{A}$ is the London equation.

Together with Ampere's law ($\nabla \times \vec{B} = \mu_0\vec{j}$) allows us the London equation (Eq.7.9) now to set up a differential equation for the magnetic field $\vec{B}$.

$$\nabla \times \nabla \times \vec{B} = -\frac{1}{\lambda^2}\vec{B}, \qquad \text{where} \ \lambda = \sqrt{\frac{m}{\mu_0 n_S e^2}} \tag{7.10}$$

This equation can also be written as

$$\nabla^2 \cdot \vec{B} = \frac{1}{\lambda^2}\vec{B} \tag{7.11}$$

To exemplify the solution of this differential equation we look at a situation were we have a superconductor filling the space for all values $x \geq 0$ corresponding to that we have vacuum at $x < 0$. Applying now a magnetic field in the vacuum region aligned along the z-axis $\vec{B} = (0, 0, B_0)$. In this case the differential equation Eq.7.11 simplifies to

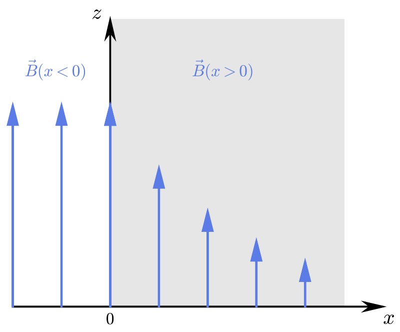

Figure 7.2: Illustration of the magnetic field decrease inside the superconductor according to Eq.7.13 . The magnetic field is pictorially drawn as blue vectors. Adapted from [2]

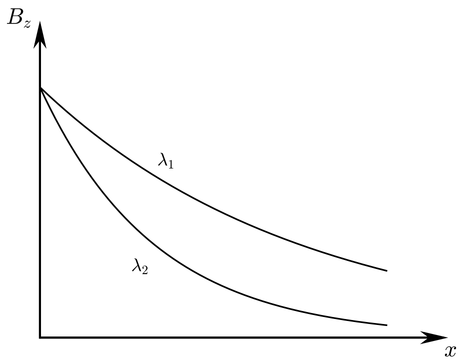

Figure 7.3: Illustration of Eq.7.13 for two different values for the London penetration depth.

$$\frac{d^2}{dx^2}B_z(x) = \frac{1}{\lambda^2}B_z(x) \tag{7.12}$$

Using the boundary conditions $B_z(x) \xrightarrow{x\to\infty} 0$ (Meissner Effect) and $B_z(x \to 0) = B_0$ leads to the solution

$$B_z(x) = B_0 e^{-x/\lambda} \tag{7.13}$$

This solution describes an exponentially decreasing magnetic field inside the the superconductor close to the surface. From this formula one can also recognize that $\lambda = \sqrt{m/\mu_0 n_S e^2}$ introduced a characteristic length scale over which the magnetic penetrates the superconductor. For that reason λ is referred to as *London penetration depth.* In 7.7 we see Eq.7.13 plotted for two different values of lambda $\lambda_1 > \lambda_2$. Looking at the definition of the London penetration depth we see that $n_{S_1} < n_{S_2}$, which means that the higher the charge density the more is the penetrating magnetic field $B_z(x)$ diminished.

7.3 Coherence Length

Another length scale that helps us to classify the different types of superconductors is the *coherence length* ξ. The coherence length is a measure of the distance within which the superconducting electron concentration cannot change drastically in a spatially-varying magnetic field.

$$\xi = \frac{\hbar v_F}{\pi \Delta} \tag{7.14}$$

Where v_F stands for the Fermi velocity and Δ for superconducting gap being present at the Fermi surface in the SC state. ξ is a parameter in the *Ginzburg-Landau Theory* and can be derived there.

The two length scales, penetration depth and coherence length, allow us now, to categorize the superconductors in the groups *Type 1* and *Type 2*. This goes as follows:

By defining $\kappa \equiv \lambda/\xi$ we say a Superconductor belongs to the group of *Type 1* (*Type 2*) if $\kappa \;<\; (>)\; 1/\sqrt{2} \simeq 0.707$.

Values of κ for some materials are given in length scale table. The classification of SC into Type 1 and Type 2 does not fully coincide with the classification of conventional and unconventional. Although a lot of the conventional (elementary) superconductors are of Type 1, there are also some exceptions like Niobium (Nb) which is a conventional Type 2 Superconductor.

include table from PPP

7.4 Ginzburg-Landau Theory

The Landau Theory of Phase Transition can also be used in the case of the transition from normal to superconducting state. The free energy per volume of the system in the superconducting state is given as

$$f_{\mathrm{SC}} \;=\; f_{\mathrm{NS}} \;+\; a(T)|\psi(T)|^2 \;+\; \frac{1}{2}b(T)|\psi(T)|^4 \;+\; ... \tag{7.15}$$

$|\psi|$ is treated as the order parameter. To find the temperature dependence of the free energy per volume we make the following assumptions: near the transition temperature T_C, the coefficient a has to be linear in temperature ($a(T) = a_0(T - T_C) + ...$) and the coefficient b has to be given as $b(T) = b_0 + ...$ with a_0, b_0 being constants and larger than zero.

Looking for the extrema of $(f_{\mathrm{SC}} - f_{\mathrm{NS}})$

$$\frac{d(f_{\mathrm{SC}} - f_{\mathrm{NS}})}{d|\psi|} \;=\; 2|\psi|\left\{a(T) \;+\; b(T)|\psi|^2\right\} \;\stackrel{!}{=}\; 0 \tag{7.16}$$

We find the following condition for $|\psi|$ to minimize $(f_{\mathrm{SC}} - f_{\mathrm{NS}})$

$$|\psi| \;=\; \begin{cases} 0, & T > T_C \\ \pm\sqrt{-a(T)/b(T)}, & T < T_C \end{cases} \tag{7.17}$$

Plugging Eq.7.17 into Eq.7.15 leads to

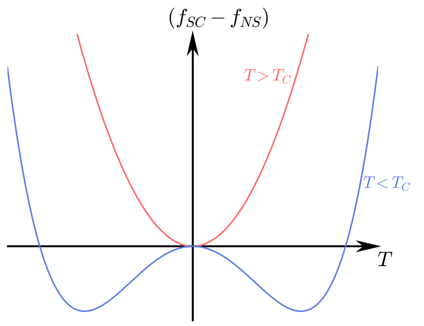

Figure 7.4: Difference of the free energy per volume between the normal- and superconducting state.

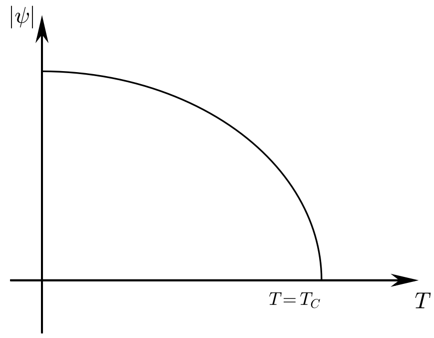

Figure 7.5: Temperature dependence of the order parameter $|\psi|$.

$$(f_{\mathrm{SC}} - f_{\mathrm{NS}}) \;=\; -\frac{a^2(T)}{b(T)} + \frac{1}{2}\frac{a^2(T)}{b(T)} \;=\; -\frac{1}{2}\frac{a_0^2(T - T_C)^2}{b_0} \tag{7.18}$$

Since f_{SC} is the free energy, we can write the entropy per volume s and the heat capacity C as

$$s \;\equiv\; -\frac{df}{dT} \qquad \text{and} \qquad C \;\equiv\; T \cdot \frac{ds}{dT} \tag{7.19}$$

This gives for the difference in the heat capacity

$$\Delta C \;\equiv\; C_{\mathrm{SC}} - C_{\mathrm{NS}} \;=\; -T_C \frac{d^2(f_{\mathrm{SC}} - f_{\mathrm{NS}})}{dT^2} \;=\; T\frac{a_0^2}{b_0} \tag{7.20}$$

Evaluating Eq.7.20 at the transition Temperature gives us the jump in specific heat at the phase transition

$$\Delta C(T_C) \;=\; \frac{a_0^2}{b_0} T_C \tag{7.21}$$

7.4.1 Orderparameter in the Ginzburg-Landau Model

To point out the connection between the penetration depth resulting from the London Equation and the Ginzburg-Landau Theory, we look a bit closer at the order parameter $|\psi|$. Before we defined the term of the super electrons n_s in the London's theory. In BCS-Theory this quantity is referred to as density of cooper pairs.

$$n_S \;=\; \begin{cases} \#\text{super electrons} & \leftarrow \quad \text{London Theory} \\ \#\text{cooper pairs} & \leftarrow \quad \text{BCS Theory} \end{cases}$$

Here we assign

$$n_S \quad = \quad 2|\psi|^2 \quad = \quad 2\frac{a_0(T_C - T)}{b_0} \tag{7.22}$$

This allows us now to express the penetration depth λ from Eq.7.10 as explicitly temperature dependent

$$\lambda(T) \quad = \quad \sqrt{\frac{b_0 m}{2\mu_0 e^2 a_0(T_C - T)}} \tag{7.23}$$

7.5 Classification of different superconductors

7.6 Vortices

To define the appearance of vortices from Type 2 Superconductors into our formalism we define the free energy per volume as

$$f_{\mathrm{SC}} - f_{\mathrm{NS}} \quad \simeq \quad a(T)|\psi(r)|^2 \; + \; b(T)|\psi(r)|^4 \; + \; \frac{\hbar^2}{2m}|\nabla\psi|^2 \tag{7.24}$$

To get the total Free energy we integrate Eq.7.24 over all space

$$F_{\mathrm{SC}} - F_{\mathrm{NS}} \quad = \quad \int d^3r(f_{\mathrm{SC}} - f_{\mathrm{NS}}) \tag{7.25}$$

We are interested now in finding the wave function $\psi(r)$ for which the Free energy is minimized. Since $\psi(r)$ is a function, this condition is formulated in a functional of the following form

$$\frac{\delta F_{\mathrm{SC}}}{\delta\psi(r)} \quad \stackrel{!}{=} \quad 0 \tag{7.26}$$

This is a differential equation for $\psi(r)$. In one dimension this DEG looks like the following

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} \; + \; a(T)\psi(x) \; + \; b(T)\psi^3(x) \quad = \quad 0 \tag{7.27}$$

A solution to this differential equation is

$$\psi(x) \quad = \quad \psi_0 \tanh\left(\frac{x}{\sqrt{2}\xi(T)}\right) \tag{7.28}$$

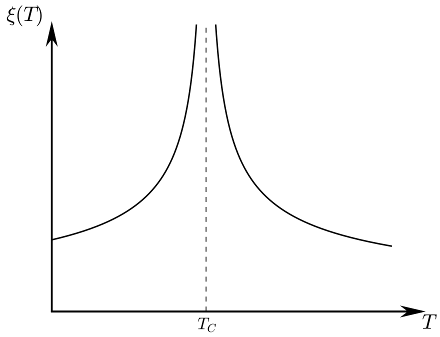

Figure 7.6: Coherence length $\xi(T)$ plotted over Temperature according to Eq.**??** . Noteworthy is the diverging of ξ when going close to T_C.

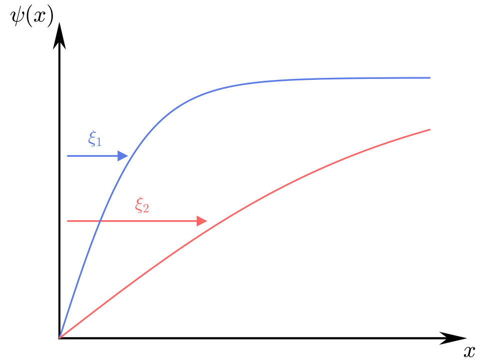

Figure 7.7: Wave function in one dimension according to Eq.7.28 . Comparing the blue and red curves shows that the wave function gets *pushed down* for increasing coherence length ($\xi_2 > \xi_1$).

The coherence length $\xi(T)$ introduces a temperature dependent length scale and is given as

$$\xi(T) \quad = \quad \left(\frac{\hbar}{2m|a(T)|}\right)^{1/2} \quad = \quad \xi_0 \ t^{-1/2} \qquad \text{with} \quad t = \frac{T - T_C}{T_C} \tag{7.29}$$

Here we used the same expression for $a(T)$ as in the Ginzburg-Landau Theory.

We can now use our expressions for the penetration depth (Eq.7.23) and the coherence length (Eq.7.29) to express the Ginzburg-Landau parameter κ as

$$\kappa \quad \equiv \quad \frac{\lambda(T)}{\xi(t)} \tag{7.30}$$

Since the temperature dependence of both characteristic length scales cancels out, κ **is independent of** T.

Each vortex has one flux quantum Φ_0. The diameter of a vortex is given by the coherence length ξ. Looking at a cut through a superconductor with edge length L, we can define the total surface of the material covered by vortices as

$$2\pi\xi^2 N \quad = \quad A_{\text{vortex}} \tag{7.31}$$

where N is the number of vortices in the material. Looking for the situation where $A_{\text{vortex}} = L^2$ we can say, that the superconducting state is fully repressed by the vortex inherent magnetic field. The magnetic field inside the superconductor can then be written as

$$H \quad = \quad \frac{N\Phi_0}{L^2} \tag{7.32}$$

This allows us to set up a relation between the upper critical field H_{c_2} for which the superconducting state is entirely suppressed and the coherence length, which defines the vortex diameter

$$H_{c_2} \simeq \frac{\Phi_0}{2\pi\xi^2} \tag{7.33}$$

Since one vortex has exactly one flux quantum, we can set up a relation between the penetration depth λ and a lower critical field H_{c_1}. This lower critical field marks the point when vortices start to be *produced* at the materials surface. We assume, that the magnetic field penetration the superconductor has at least to be as strong as one flux quantum to be able to create a vortex

$$\pi\lambda^2 H \stackrel{!}{=} \Phi_0 \qquad \Rightarrow \qquad H_{c_1} = \frac{\Phi_0}{\pi\lambda^2} \tag{7.34}$$

sketch - vortices in the material

sketch - condition for creating one vortex

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