Electron-hole excitations in a ring driven by a time-dependent Aharonov-Bohm-flux

Bachelor's Thesis

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Abstract

Through the Aharonov-Bohm effect an electron can be influenced by a magnetic flux without being in contact with a magnetic field. This thesis studies a Fermi sea in a ring that is threaded by a magnetic field. We will discuss the influence of changing the magnetic flux has on the energy spectrum of the electrons. We will also introduce a perturbation in form of a δ *potential. We use analytical tools like the Landau-Zener formula, as well as numeric simulations of the (time dependent) Schrödinger equation. Lastly we will transform our findings into the electron-hole picture.*

Contents

Chapter 1

Introduction

1.1 Setup

In this thesis we will discuss electron and electron-hole excitations fundamentally caused by the Aharonov-Bohm effect.
We start with a ring of radius R and consequently circumference $C = 2\pi R$. The coordinate x describes the path along the ring, starting at $x = 0$ and going to $x = C$ anti clockwise. In the ring we put an odd number of electrons (one ore more). An electrons is a quantum-mechanical particle and can be described with a wave function. The wave function has to be continuous. In a ring specifically, that also means periodical boundaries, $x = 0 = C$.
We construct a variable magnetic field $B = \nabla \times A$, that goes through the enclosed area of the ring. At the ring itself, the magnetic field is 0. However, the electromagnetic potential A[1] does not have to be 0.
At $x = \frac{C}{2}$ there is a perturbation in the form of a δ potential of the height γ.
A similar system, on a infinitive long line but with also periodic potentials has been discussed by Baym [1].

[1] A is a vector field (as well as B) but we do not write the vector array, since we are only interested in the value on the ring, in one dimension.

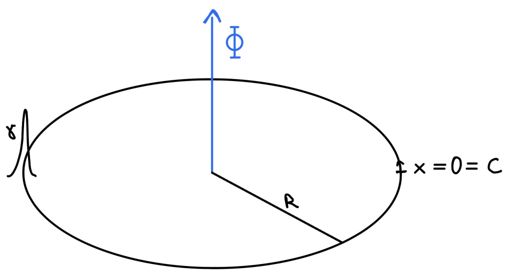

Figure 1.1: The setup of our system. A ring with the radius R and the circumference C. At $x = \frac{C}{2}$ the is a δ potential. Through the ring goes the magnetic flux Φ.

The Hamiltonian of this system is

$$H = \frac{(p + \frac{e}{c}A)^2}{2m_e} + \gamma\delta\left(x - \frac{C}{2}\right). \tag{1.1}$$

The first term describes the electron interacting with the electromagnetic potential. p is the canonical momentum of the electron. The electron has a negative charge of $q = -e < 0$ and a mass of m_e. We are using Gaussian units, c is the speed of light in vacuum. The squared bracket links the momentum and the electromagnetic potential together.
The second term describes the artificial δ potential.

1.2 Chapter Overview

In this Chapter, we look at the for this system fundamental Aharonov-Bohm effect. Changes in the magnetic flux inside area of the ring influence the energy of the electrons on the ring.

Chapter 2 attends to the energy spectra of the system. We consider two cases. A rapid change in the magnetic flux enables the electrons to tunnel through the potential barrier of the δ function. For the first case we can anticipate, that the energy spectrum behaves as if there where no potentials. Therefore, we solve the stationary Schrödinger equation for a adjusted Hamiltonian. We can use the outcome of this case to determine the energy spectrum for infinitesimal slow changes of the magnetic flux. Instead of solving the Schrödinger equation analytically, we use numeric simulation and nearly degenerate perturbation theory to adjust the energy spectrum. In the second case, energy bands are formed. We determine the relation between the band gaps and the potential γ.

In Chapter 2 we have determined two partly different energy spectra for essentially very rapid and very small changes of the magnetic flux. In Chapter 3 we focus on determine the course of the transition between the two cases. The Landau-Zener formula is discussed. it describes the tunnel probability of one electron at an energy gap. These results are compared to the numeric solution of the time-dependent Schrödinger equation of the system.

The results from the former Chapters have been expressed in probabilities of occupied electron states. Chapter 4 introduces the electron-hole picture. Any influence changes in the magnetic flux have on the Fermi sea are exclusively expressed through the creation of an electron-hole pair. Lastly, we follow this transition by contextualizing the results in a more approachable environment. We determine the consequences on the current in the ring for the different scenarios.

1.3 Aharonov-Bohm effect

In this section, we introduce the Aharonov-Bohm effect in relation to our specific setup. As mentioned above, we chose our setup so that the magnetic field $B = \nabla \times A$ is non existing everywhere on the Ring. That is not necessary true for the electromagnetic potential A, featured in the Hamiltonian (1.1). The electromagnetic potential on the ring is connected to the magnetic flux inside the enclosed area. We find

$$\Phi = \int BdF = \int_0^C A(x)dx \tag{1.2}$$

with Stokes' theorem. Here, F describes the area of the circle inside the ring. x is the position on the ring and lives between 0 and the circumference C. The magnetic flux is effected by changes in the magnetic potential.

Using the Gauge transformation, we can adjust any electromagnetic potential A to be constant on the ring. In consequence, the wave function of the electron is only altered by a phase, which is discussed in the Appendix A. In the case of constant A our setup is symmetric with respect to the center of the ring. The Noether theorem then predicts a conserved quantity. The Appendix B shows, it is the canonical angular momentum P_ϕ, that is conserved. This is also true if $A(t)$ changes with time, but stays constant in x in the process.

We compare that to the kinetic angular momentum $L_{kin}(t) = P_\psi R + \frac{e}{c}A(t)R$. $L_{kin}(t)$ always permutes with the Hamiltonian $H(t) = \frac{L^2_{kin}(t)}{2m_e R^2}$. However, the total time derivative of L_{kin}

$$\frac{d}{dt}L_{kin} = i[H(t), L_{kin}] + \partial_t L_{kin} = 0 + \frac{e}{c}R\dot{A} \tag{1.3}$$

is not equal to 0, for a time dependent electromagnetic potential. The kinetic angular momentum is not conserved and changes with the magnetic flux.

Overall, if we increase the electromagnetic potential A is generally attended by an increase in the magnetic flux Φ. A change in A simultaneously induces a change in the time derivative of the angular momentum. Therefore, a change in the magnetic flux influences the energy of any electron in the ring.
The phenomenon is named Aharonov-Bohm effect [4]: Changes in the electromagnetic potential can be enough to influence a charged particle even in magnetic free space.

Chapter 2

Energy spectrum of the ring

In this chapter, we solve the stationary Schrödinger equation for an electron moving on a ring threaded by a magnetic field. We will use the results to determine the energy spectrum of the Hamiltonian after a small δ potential added to the ring. The δ potential leads to scattering and backscattering.

2.1 Spectrum without δ scattering

We will study the Hamiltonian

$$H = \frac{(p + \frac{e}{c}A)^2}{2m_e} \tag{2.1}$$

of an electron on the ring, without any additional potential. $p = -i\hbar\partial_x$ is the canonical momentum of the electron and A is the electromagnetic vector potential. We can find the wave function for the special case $A' =$ const. along the ring first. We can use the information from the Appendix A to rewrite it for any smooth electromagnetic potential using the gauge transformation

$$A \to A' = A(x) + \partial_x \chi(x). \tag{2.2}$$

The transformed electromagnetic potential resolves in a different Hamiltonian $H' = \frac{(p+\frac{e}{c}A')^2}{2m_e}$.

We can solve the stationary Schrödinger equation

$$H'\Psi'(x) = E\Psi'(x) \tag{2.3}$$

and obtain the wave function

$$\Psi'(x) = e^{-i\frac{e}{c}A'x}\left[c_1 e^{i\sqrt{2m_e E}x/\hbar} + c_2 e^{-i\sqrt{2m_e E}x/\hbar}\right]. \tag{2.4}$$

c_1 and c_2 are arbitrary. Since the ring is symmetric and periodic, we only need to consider either the forwards or backwards travelling electron. Therefore, we can set $c_1 = 0$. Using the phase $e^{i\frac{e}{c}\chi(x)/\hbar}$ from the gauge transformations [1], this leads to the wave function

$$\Psi(x) = c_2 e^{-i\frac{e}{c}\int_0^x A(x)dx} e^{-i\sqrt{2m_e E}x/\hbar} \tag{2.5}$$

for any $A(x)$.

On a ring, we assume a continuous wave function of the electron. This is expressed in the boundary condition

$$\Psi(0) = \Psi(C) \tag{2.6}$$

where C is the circumference of the ring. Solving for the energy gives us

$$E(n) = \frac{2\pi^2\hbar^2}{m_e C^2}(n - \frac{e}{2\pi c}\Phi)^2. \tag{2.7}$$

There are different states for the electron labeled by $n \in \mathbb{Z}$. Every state has a discrete energy. The term $\frac{e}{2\pi c}\Phi$ will be written in the following as n_Φ. One n_Φ is labeled a flux quantum. As seen in fig. 2.1, at n_Φ the energy spectrum looks the same as at $n_\Phi + 1$.
For an electron in a fixed state, there is a parabolic relation between the magnetic flux and the energy of the electron. The individual states n only differ with regards to the magnetic flux at their roots.

We consider a setup with more than one electron. For simplification, we treat the electrons as spinless. For more than one electron in the system the Pauli principle dictates that each particle occupies a different state. That means that every state n is only occupied by at most one electron. In the ground state of the system, we end up with a Fermi sea where all the lowest energy states are filled. For example, 5 electrons in $n_\Phi = 0$ (figure 2.1) occupy $n = 0, -1, 1, -2, 2$. The highest energy for any of these electrons, in this case $E(n = 2)$ is called the Fermi energy.
For now, the state of each electron is fixed. If we change the magnetic flux from the ground state at $n_\Phi = 0$ to $n_\Phi = 1$, we will see that the energy of every single electron has changed. In our former example it would seem as if we looked at the $n_\Phi = 0$ spectrum with electrons in the states $n = 1, 0, 2, -1, 3$. The energy $E(n = 3)$ in particular is higher than the Fermi energy. It should be noted that electrons are indistinguishable from each other. We can only observe which states are occupied not by which electron.

[1] and $\chi(x) = -\int_0^x A(x')dx' + A'x + \chi_0$

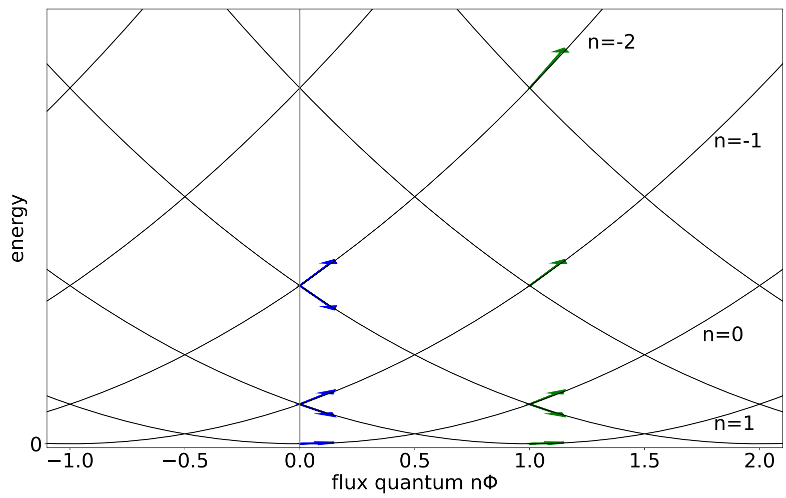

Figure 2.1: Energy spectrum of an electron on the ring without δ potential. The individual states follow the form of a parabola with a low point of $E = 0$ and n_Φ next to each other. The blue arrows represent the lowest 5 occupied states at $n_\Phi = 0$. States above $E = 0$ are degenerated for every $n_\Phi = \mathbb{Z}$. One state is maintained by following the line. In green, the energy of the previously blue states at $n_\Phi = 1$ are marked.

2.2 Spectrum with scattering

Next, we breach the rotational symmetry by introducing a δ potential at the coordinate $x = \frac{C}{2}$. The corresponding Hamiltonian was introduced in Chapter 1. The wave function on the ring is

$$\Psi(x) = \begin{cases} ae^{ikx} + be^{-ikx}, & x < \frac{C}{2}, \\ Ae^{ikx} + Be^{-ikx}, & x > \frac{C}{2} \end{cases} \tag{2.8}$$

with $k = \sqrt{2m_e E}/\hbar$. Unlike Chapter 2.1, an electron has the potential to be scattered and change direction. Therefore both positive and negative momentum k have to be accounted for simultaneously. After also multiplying with the factor $e^{i\frac{e}{c}\int_0^x A(x)dx}$, the wave function is still continuous everywhere in the ring, except for $x = \frac{C}{2}$ and $x = 0$. This is fulfilled in both sections of (2.8). Between the sections the two boundary conditions

$$\begin{aligned} a + b &= e^{-i\frac{e}{c\hbar}\Phi}\left(Ae^{ikC} + Be^{-ikC}\right), && \text{for } \Psi(0) = \Psi(C) \\ B - b &= (a - A)e^{ikC}, && \text{for } \Psi\left(\frac{C^-}{2}\right) = \Psi\left(\frac{C^+}{2}\right) \end{aligned} \tag{2.9}$$

express this requirement. Furthermore, the first derivative is also continuous everywhere on the ring (including at $x = 0$) except at $x = \frac{C}{2}$. We can calculate the jump in the derivative

$$\begin{aligned}
&\lim_{\epsilon\to 0}\int_{\frac{C}{2}-\epsilon}^{\frac{C}{2}+\epsilon} H\Psi(x)dx\\
=&\lim_{\epsilon\to 0}\left[-\frac{\hbar^2}{2m_e}\int_{\frac{C}{2}-\epsilon}^{\frac{C}{2}+\epsilon}\frac{\partial^2}{\partial x^2}\Psi(x)dx+\gamma\int_{\frac{C}{2}-\epsilon}^{\frac{C}{2}+\epsilon}\delta\left(x-\frac{C}{2}\right)\Psi(x)dx\right]\\
=&\lim_{\epsilon\to 0}\left[-\frac{\hbar^2}{2m_e}\left(\partial_x\Psi\left(\frac{C}{2}+\epsilon\right)+\partial_x\Psi\left(\frac{C}{2}-\epsilon\right)\right)+\gamma\Psi\left(\frac{C}{2}\right)\right]\\
=&\lim_{\epsilon\to 0}E\int_{\frac{C}{2}-\epsilon}^{\frac{C}{2}+\epsilon}\Psi(x)dx
\end{aligned}\tag{2.10}$$

using the Schrödinger equation. We end up with the additional two conditions

$$\begin{aligned}
&a-b=e^{-i\frac{e}{c\hbar}\Phi}\left(Ae^{ikC}-Be^{-ikC}\right), && \text{from } \Psi'(0)=\Psi'(C)\\
&(a-A)e^{ikC}+B-b=i\frac{2m_e\gamma}{k\hbar^2}(Ae^{ikC}+B), && \text{from } \Psi'\left(\frac{C^+}{2}\right)-\Psi'\left(\frac{C^-}{2}\right)=\frac{2m_e\gamma}{p\hbar^2}\Psi\left(\frac{C}{2}\right).
\end{aligned}\tag{2.11}$$

In total, we have four equations for the five variables a,b,A,B and k. If we solve this set of equations, we end with one equation

$$0=\frac{\hbar^2k}{m_e\gamma}\cos kC-\frac{\hbar^2k}{m_e\gamma}\cos\frac{e}{c\hbar}\Phi+\sin kC \tag{2.12}$$

for k.
We divide by $\frac{\hbar^2k}{m_e\gamma}$, in the case $k\neq 0$. If we then separate the terms depending on k, we see that they equal $\cos\frac{e}{c\hbar}\Phi$, which only lives between -1 and 1. This restricts the possible values of k. Since $E=\frac{\hbar^2k^2}{2m_e}$ the energies that can be attained by the electron are restricted as well. More precisely energy bands and energy gaps form in the spectrum. We can calculate the with of these gaps using the nearly degenerate perturbation theory (Appendix C).

If we write the Hamiltonian from Chapter 1 as $H=H^{(0)}+H^{(1)}$ then $H^{(1)}$ equals $\gamma\delta\left(x-\frac{C}{2}\right)$. The nearly degenerate perturbation theory only works for very small γ (more precise approximation in Chapter 2.3) where we can assume the proportionality between energy gap and γ is linear.
We will assume the circumference of the ring is $C=2\pi$. That makes $\sin(kC)=\sin[(k+1)C]$ and $\cos(kC)=\cos[(k+1)C]$. The gaps in k will be separated by 1 as well. We look at the crossing between the states (k and $k-1$)

$$\Psi_0(x)=e^{-i\frac{e\Phi}{2\pi c\hbar}x\pm ikx} \tag{2.13}$$

and

$$\Psi_{-1}(x)=e^{-i\frac{e\Phi}{2\pi c\hbar}x\pm ikx-ix} \tag{2.14}$$

that are only separated by the band gap at $\Phi=0$. We calculate the off diagonal matrix element

$$\frac{1}{2\pi}\int\Psi_0^*(x)H^{(1)}\Psi_{-1}(x)dx=\frac{1}{2\pi}\int\gamma\delta\left(x-\frac{C}{2}\right)e^{-ix}dx=-\frac{\gamma}{2\pi}. \tag{2.15}$$

The phase in the integral depends on the position of the δ potential on the ring. The band gap amounts to the double

$$\Delta = \frac{\gamma}{\pi} \tag{2.16}$$

of this matrix element.

2.3 Numeric calculation of energy bands

We will solve (2.12) numerically using the method of bisection. We know the equation can be solved for every Φ by an infinite number of k. Therefore, our goal is to find the roots of

$$f(k) = \frac{\hbar^2 k}{m_e \gamma} \cos kC - \frac{\hbar^2 k}{m_e \gamma} \cos \frac{e}{c\hbar}\Phi + \sin kC \tag{2.17}$$

for every Φ. This function is continuous. If Φ is set and two different k have a positive and a negative outcome, there has to be an outcome of 0 in between. We know for $\gamma = 0$ and $\Phi = 0$ this requirement is fulfilled at $k = \frac{2\pi}{C}n$. Assuming a small change in γ or Φ only results in a small change in k, we chose the intervals $\frac{2\pi}{C}(n \pm \frac{1}{2})$ centered around this k value. If the signs of $f(k)$ of the boundaries are different, we half the interval. At least one of the two new intervals has to have a zero point. We proceed with this method for 10 iterations. After that, for every interval that has a zero point inside, we assume the first boundary is a close approximation to the actual k value of the zero point.

In fig. 2.2, the respective energy spectrum is shown. Note that the energy is proportional to k^2. The original parabolic form is split by band gaps where crossing between states used to be. These gaps get bigger with increased potential γ, for $\gamma < \frac{0.1\hbar C}{2\pi m_e}$ in a linear manner.
We are interested in the proportionality factor between the width of the energy gaps and the potential. We can get the k values that do not fulfill equation (2.12) from our data. We square the k values at both limits (one under, one above) of the gap and then take the difference Δk^2. The Δk^2 do not show a significant difference between gaps. If we do this for a variety of γ we find for the energy difference

$$\Delta E = \frac{\hbar^2}{2m_e}\Delta k^2 \approx 0.3\gamma \tag{2.18}$$

that the proportionality factor comes close to the analytical predicted $\frac{1}{\pi}\gamma$ from Section 2.2.

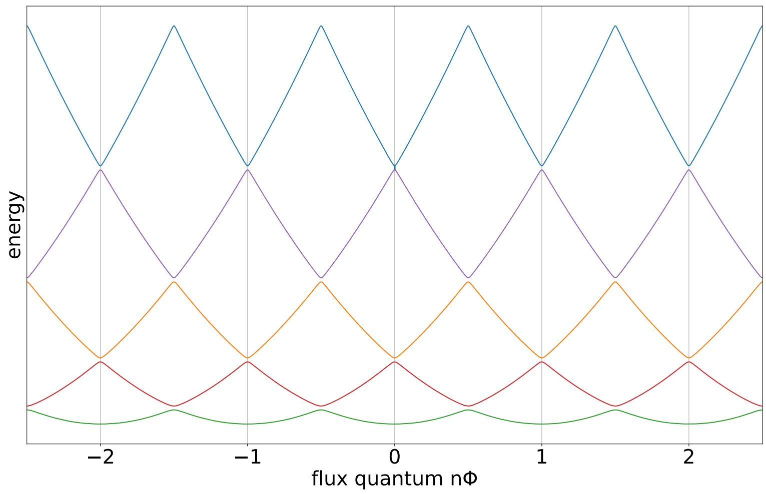

Figure 2.2: Energy spectrum of the ring with the potential $\gamma\delta\left(x-\frac{C}{2}\right)$. C is assumed to be 2π and $\gamma=\frac{0.1\hbar}{m_e}$. A band structure forms with energy gaps proportional to γ, separating different energy levels.

Chapter 3

Excitation of the Fermi sea

The energy spectrum from Sections 2.2 and 2.3 are the static solutions to the time independent Schrödinger equation. In this Chapter we will see, that the spectrum from section 2.1 (Hamiltonian without δ potential) will be the solution for a very rapid changing magnetic flux, even with added δ potential [1]. We will now focus on a dynamic approach and want to find the quantitative transition between these two extremes.
In this Chapter, the magnetic flux will be time dependent. We find that the corresponding time-dependent Schrödinger equation can only be solved numerically. For an alternative approach, we can use the Landau-Zener formula instead. It will be explained in the following Section.

3.1 Landau-Zener tunneling in a ring

In Section 2.3 we found an energy spectrum containing energy bands. The difference to the spectrum from Section 2.1 is everywhere where a crossing in 2.1 was, is an band gap in 2.3. This can be seen in Figure 3.1. If the energy band gaps are small, there is a probability with which an electron tunnels through a crossing, when the magnetic flux is changed around the crossing. Tunneling means in this case, the electron will occupy an band of higher energy. The probability of one electron tunneling through one crossing is expressed in the Landau-Zener formula

$$P_{LZ} = e^{-\frac{\pi\Delta^2}{4\hbar\alpha v}}. \tag{3.1}$$

Δ is the band gap. It is given by the Hamiltonian and equation (2.16). The wider it is, the less likely an electron changes energy bands. v is the rate of the change in the electromagnetic potential (magnetic flux). For linear increase that is simply $A(t) = vt$. The faster the crossing is approached, the more likely an electron will tunnel. Lastly, α is the slope of the relevant crossing.
For the slope of the energy we are interested in the linear term of the spectrum

$$\partial_{n_\Phi} E = -\frac{4\pi^2\hbar^2}{m_e C^2}(n - n_\phi). \tag{3.2}$$

[1] Sudden approx.

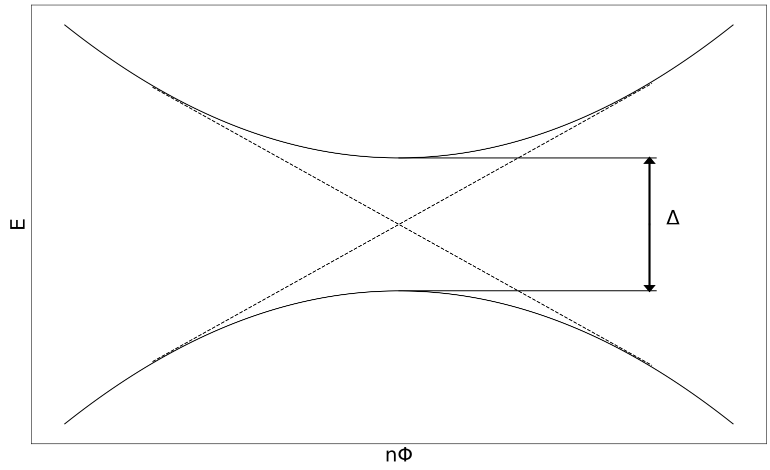

Figure 3.1: Exemplary representation of an energy gap. The solid lines are the energy bands. The have a minimal difference (energy gap) of Δ towards each other. The dotted lines are the previous crossings. If n_Φ is raised fast enough, an electron will follow their path instead.

We do not only look at singular electron crossings, but a Fermi sea. In a Fermi sea all states with energies lower than the Fermi level are occupied. Therefore, a crossing of 2 energy bands includes 2 occupied states. The probability, that an electron from the lower band tunnels into the higher band is the same as the reverse. Since we do not distinguish between electrons, the probability of each state being occupied by one electron after the crossing is 1.
Instead we are more interested in the crossings of electrons on the surface of the Fermi sea. In the ground state of the system there are only two electrons that fulfill this condition. We can use the Landau-Zener formula to look at them separately from the rest.
Exemplary we examine the first crossing at $n_\Phi = \frac{1}{2}$. m is the number of electrons in the system. The state with the highest energy that is occupied at the crossing is $n = -\frac{m}{2} + \frac{1}{2}$. The energy spectrum has a slope of

$$\alpha = \frac{2\pi^2\hbar^2}{m_e C^2} m \tag{3.3}$$

We take note that the slope α depends on the number of electrons in the system. The higher the number of occupied states, the steeper the crossing at Fermi energy levels becomes. In the Landau-Zener formula steeper slope coincides with a raised probability to tunnel.
For simplicity we also set $C = 2\pi$, $2m_e = \hbar = \frac{e}{c} = 1$, and $\Delta = \frac{\gamma}{\pi}$. The probability is

$$P_{LZ} = e^{-\frac{\gamma^2}{4\pi m v}} \tag{3.4}$$

for an electron to tunnel along the highest energetic crossing.
For example we look at 5 electrons, with $v = 10^{-6}$ and $\gamma = 0.01$ and a magnetic flux between $n_\Phi = 0$ and $n_\Phi = 1$. The highest energetic electron occupies the state $n = -2$. It tunnels with the probability of $P_{LZ} = 0.85$ through the δ potential. With the probability of $1 - P_{LZ} = 0.15$ it does not tunnel and instead of state $n = -2$ occupies state $n = 3$.

We increase the magnetic flux from 0 to nearly 1. Every electron interacted with one crossing. States scarcely under the Fermi energy may not be occupied anymore. States just over the Fermi energy might however. If we increase the magnetic flux further the interference of probabilities gets more complicated.
For higher magnetic flux there is a crossing every $\frac{1}{2}n_\Phi$. Every crossing an additional possible state may be occupied, as shown in fig. (3.6). The new states for a positive magnetic flux are always of a positive state number n. In the Figure black dots indicate, that this state is definitely occupied. Crossings between states at lower energy levels f.e. between $n = 0$ and $n = 3$ at $n_\Phi = \frac{3}{2}$ have a low chance of tunneling. If the slope at the crossing is higher, the probability of a Landau-Zener tunneling is increased. Therefore, f.e. the crossing between $n = -2$ and $n = 3$ at $n_\Phi = \frac{1}{2}$ is higher than the prior.

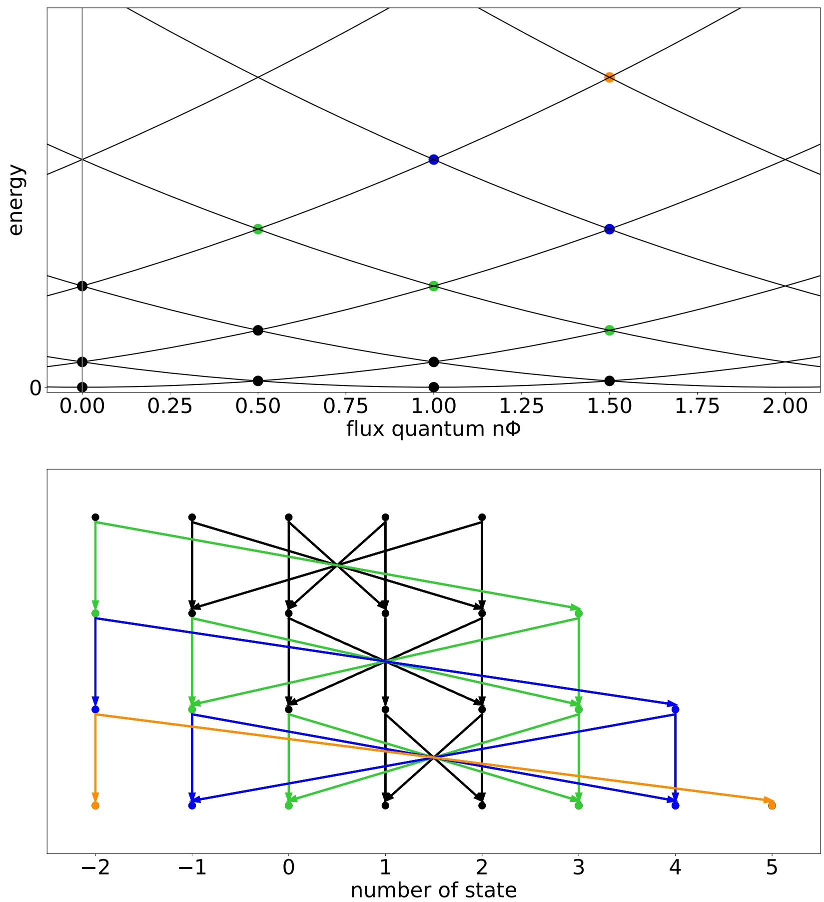

Figure 3.2: Above: We can see all possibly occupied electron states fat $n_\Phi = 0, \frac{1}{2}, 1, \frac{3}{2}$. The black dots are definitively occupied by an electron. The green dots have to tunnel through an energy gap once, the blue dots twice, and the orange dot three times. Beneath: The corresponding possibilities, for each electron, if we assume we can follow each electron separately. The top row represents the system at $n_\Phi = 0$. Every step down is another crossing. For example, an electron at the orange dot in the Figure above could follow the path down at $n = 5$, or up at $n = 2$. It is only possible to increase the number n, for a positive magnetic flux.

3.2 Simulation of the time-dependent Schrödinger equation

We are interested in the energy spectrum when $A(t)$ changes with the time. In this section, we want to simulate the time development of the wave functions of the hole system. We can describe the system with the time-dependent Schrödinger equation

$$-i\hbar\partial_t\Psi(x) = H(t)\Psi(x) \tag{3.5}$$

where as stated $A(t)$ is time dependent. We can write the time derivative as

$$i\hbar\frac{\Psi_{j+1}-\Psi_j}{\delta} = H\Psi_j \tag{3.6}$$

with the step width δ. Ψ_j is the wave function before, Ψ_{j+1} after the step. We want to solve the equation for Ψ_{j+1} and continue an iterative progress numerically. Notice, that the term $\mathbb{1} - i\frac{\delta}{\hbar}H$ is not necessary unitary. We need to perform unitary action, because it preserves the orthogonality of the electron states. So instead we use

$$\Psi_{j+1} = \frac{\mathbb{1} - i\frac{\delta}{2\hbar}H}{\mathbb{1} + i\frac{\delta}{2\hbar}H}\Psi_j. \tag{3.7}$$

The fraction is unitary, if H hermitian. We calculate the first element of its Taylor series $\mathbb{1} - 2i\frac{\delta}{2\hbar}H$. This is the term we initially wanted. Therefore, we get

$$(\mathbb{1} + i\frac{\delta}{2\hbar}H)\Psi_{j+1} = (\mathbb{1} - i\frac{\delta}{2\hbar}H)\Psi_j. \tag{3.8}$$

We will start with a wave function $\Psi_{j=0}$. In every step act on the right side with a matrix multiplication and solve for Ψ_{j+1}. Note that we must use A_j on both sides of the equation.

Numerically, we can describe the wave function and Hamiltonian as matrices. For our system of wave functions we can separate the possible states by n

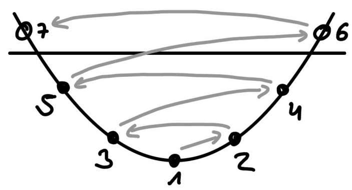

Figure 3.3: Demonstrative representation of the numbering of the electron states. Starting at the bottom of the Fermi sea and going up, alternating between positive and negative states.

value, or by k value (and therefore by energy). We chose to separate by n value, reflecting the states from Section 2.1. We construct the orthogonal basis

$$\Psi_{n,j} = c_{n,j} e^{inx}. \tag{3.9}$$

$c_{n,j}^2$ is the probability, that the state n is occupied by any electron. Thus, its value is always between 0 and 1.
The matrix at the ground state of the system is

$$\Psi_{j=0} \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \\ 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}. \tag{3.10}$$

It has $2N+1$ rows, one for each state. Only the first m states are occupied, after that every row is filled with 0s. We can't simulate the system for infinite N, but we find that $N > m$ is enough. In the matrix above states are numbered with raising energy level (fig. 3.3). If we take the matrix of probabilities (each entry squared), every row sums to the probability with which this state is occupied by any electron. There are m number of columns, each describing one electron. Each column must sum to 1, because that is the probability that this electron exists.
We can calculate the matrix elements of the Hamiltonian operator with

$$H_{nm} = \frac{1}{C} \int_0^C e^{-inx} H e^{imx} dx. \tag{3.11}$$

We split the Hamiltonian $H = \frac{(p+\frac{e}{c}A)^2}{2m_e} + \gamma\delta(x - \frac{C}{2})$ in two terms. The term $\gamma\delta(x - \frac{C}{2})$ results in an absolute value of $\frac{\gamma}{C}$ for every matrix element. This does not change, no matter how many iterations there are. The phase is not important, as we are only interested in the probabilities.
The integral over the first term can be calculated like this:

$$\begin{aligned} &\frac{1}{2m_e C} \int_0^C e^{-inx} (-\hbar^2 \partial_x^2 + i\hbar \frac{2e}{c} A(t) \partial_x + \frac{e^2}{c^2} A^2(t)) e^{imx} dx \\ =&\frac{1}{2m_e C} (\hbar^2 n^2 - 2\hbar \frac{e}{c} A(t) n + \frac{e^2}{c^2} A^2(t)) \delta_{nm}. \end{aligned} \tag{3.12}$$

We see the first term of the Hamiltonian results in diagonal matrix elements. They depend on the state (0,1,−1,2,−2,...) they interact with and the electromagnetic potential that changes with each step.
The Hamiltonian matrix is assembled into

$$H = \frac{1}{2m_e C} \begin{pmatrix} \frac{e^2}{c^2} A^2 & 0 & 0 & \cdots \\ 0 & \hbar^2 - \hbar \frac{e}{c} A + \frac{e^2}{c^2} A^2 & 0 & \cdots \\ 0 & 0 & \hbar^2 + \hbar \frac{e}{c} A + \frac{e^2}{c^2} A^2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} + \frac{\gamma}{C} \begin{pmatrix} 1 & 1 & 1 & \cdots \\ 1 & 1 & 1 & \cdots \\ 1 & 1 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{3.13}$$

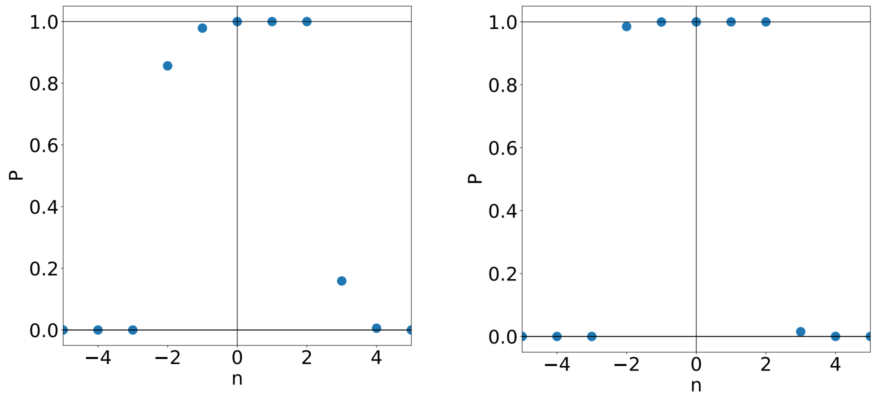

Figure 3.4: Probability P of the different states n being occupied by an electron. On the left with $v = 10^{-6}$ (Einheit?), on the right with $v = 10^{-5}$. The more rapid change of the magnetic potential A increases the probability of the states being conserved. In the case of the slower change of A the state to lose probability is $n = -2$, the state to gain probability is $n = 3$. They are on the borders of the Fermi sea, the crossing between them only includes one electron.

It has the dimensions $2N + 1 \times 2N + 1$.

In fig. 3.4 we see the results of the numeric calculation. The states $n = -1, 0, 1, 2$ are all occupied by an electron. The probability of the state $n = -2$ is decreased. The probability of state $n = 3$ is increased by the same amount. As we expected in Section 3.1, for a more rapid change in the magnetic potential, the state $n = -2$ is more likely preserved.

We also see in fig. 3.5 that after the crossing at $n_\Phi = \frac{3}{2}$ two more states are possibly occupied. Also noticeable, the state $n = 0$ has lost more probability than both its neighbouring states. This was also predicted due to the slope of the $n = 0$ to $n = 3$ tunneling being so flat.

Not only can we look at the development for longer periods of increase of the potential. We can also simulate the time evolution of one state at a specific crossing. For example we pick the crossing at $n_\Phi = \frac{1}{2}$ of the occupied $n = -2$ and the unoccupied state $n = 3$.There are only 5 electrons, so this is a crossing at the Fermi level. We can see the time evolution of both states in fig. 3.6. Both states show oscillation typically for Landau-Zener tunneling. After a decay process their probability settles on the expected value.

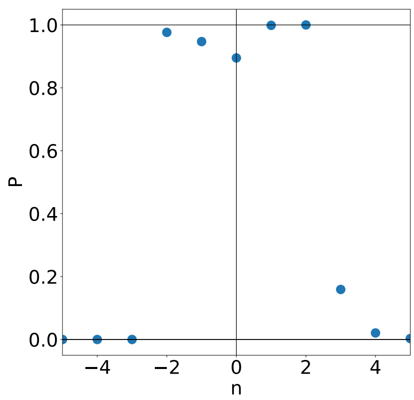

Figure 3.5: The spectrum of occupied states after increasing n_Φ from 0 to nearly 2. Noticeably, the boundary states have not lost most of the occupation probability.

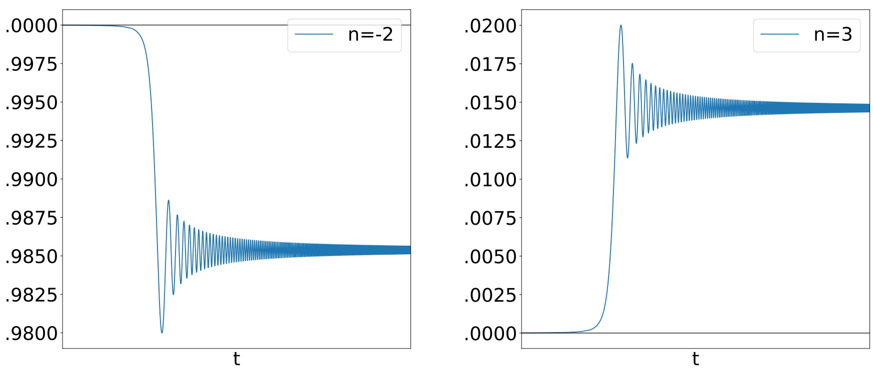

Figure 3.6: The time evolution of the probability that the states $n = -2$ (left) and $n = 3$ (right) are occupied. The probability has a transient effect, before the final value is reached.

Chapter 4

Description in terms of electron-hole excitations

In this Chapter, we will examine how the electron excitations from the previous Chapters can be described in the electron-hole picture. This will help us understand the physical consequences of our calculations.

4.1 Electron-hole picture

We have found that electrons change their occupied states if the magnetic flux is nearly statically increased. The energies overall do not change in that case. In comparison, with rapid change of the magnetic flux the electrons occupy the same states. However, every electron in the spectrum changes its energy.

Electrons changing their respective energies is specifically interesting at the Fermi level. We do not need to look at the electrons individually. Instead, we assume an electron-hole pair was created. The rest of the electrons are treated as if nothing changed energy wise.
In fig. 4.1 we see that the picture of different electrons is not so different to the electron-hole picture. We also see, that the created electron is slightly over the Fermi energy, the created hole is slightly under the Fermi energy (or on it).

The two corresponding pictures have to be equivalent. For example, an electron has a positive mass and negative charge. A hole however, has negative mass and positive charge, if we treat it as a particle. The conservation of mass and charge can not be broken.
Similarly, measuring quantities such as total angular momentum and total energy of the system have to be consistent with the separate-electrons picture as well.
Energy has already been accounted for. The total angular momentum will be discussed sec. 4.2.

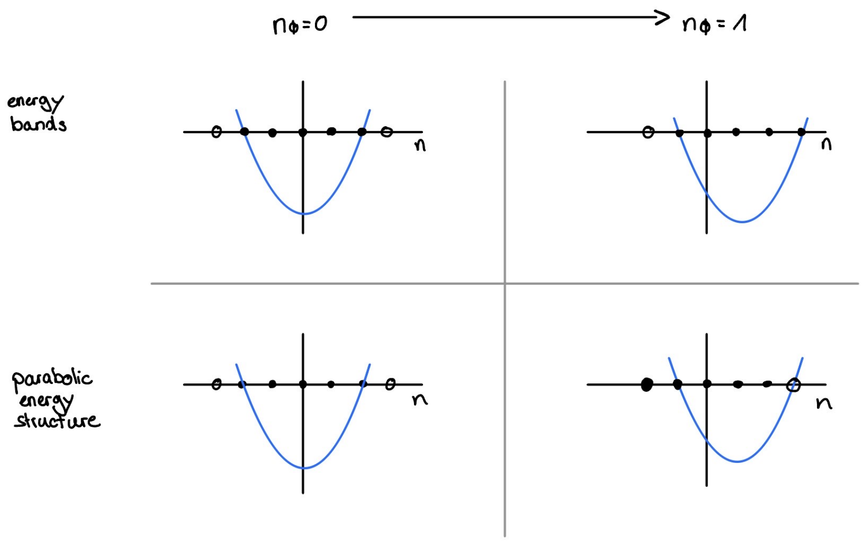

Figure 4.1: Comparison between the energy-band spectrum and the parabolic-energy spectrum in the transition from $n_\Phi = 0$ to $n_\Phi = 1$. The black dots represent the states occupied by electrons. The blue curve represents the energy these states have in the Fermi sea. The focus of the energy curve shifts to the right during the transition. With energy bands, the occupied states shift as well. However, if the transition of the magnetic flux is rapid, the states do not change. The disparity between the two has the effect of an electron-hole pair.

4.2 Physical significance

We start this section with calculating the angular momentum of the electron. The relation between the kinetic angular momentum L_{kin} and energy E is

$$E = \frac{L_{kin}^2}{2m_eR^2} = \frac{\hbar^2}{2m_eR^2}(n - n_\Phi)^2 \tag{4.1}$$

due to $C = 2\pi R$ and eq. (ref). In the ground state of the system, with $m = 5$ electrons the highest energetic states are $\pm\frac{m-1}{2}$. The -1 accounts for the state of 0 kinetic energy. The $\frac{1}{2}$ is in place because we have negative and positive state numbers n.

We know from sec. 2.1, that the energy spectrum at $n_\Phi = 0$ looks similar to $n_\Phi = 1$. This is useful, since we want to treat most of the Fermi sea as if no energy changes have happened. From the two highest energetic states only $-\frac{n+1}{2}$ increases its energy at $n_\Phi = 1$ to $\frac{\hbar^2}{2m_eR^2}(-\frac{m-1}{2} - 1)^2$. The respective angular momentum of the electron is

$$L_e = \frac{m+1}{2}\hbar. \tag{4.2}$$

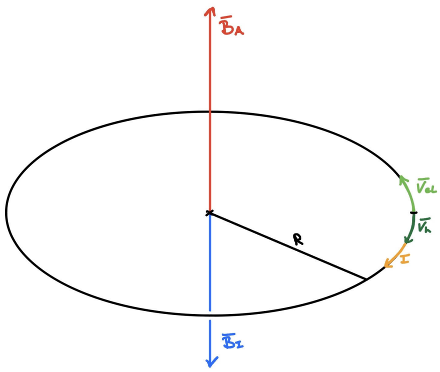

Figure 4.2:

For the electron hole we want to assume a similar energy spectrum. However, there are a few changes, for example the charge is $q = e > 0$. Therefore, in the energy spectrum of the hole $n_\Phi = \frac{e}{2\Pi c}\Phi \rightarrow n_\Phi = -\frac{e}{2\Pi c}\Phi$. With n_Φ changing its sign, we have to inverse the numbering of n. That way, the roots of the parabolic states are still in the right position.We are specifically interested in the other Fermi-energy state $\frac{m-1}{2} \rightarrow -\frac{m-1}{2}$. With the kinetic energy $\frac{\hbar^2}{2m_e R^2}(-\frac{m-1}{2}+1)^2$ we find the kinetic angular momentum

$$L_h = \frac{m-1}{2}\hbar. \tag{4.3}$$

The absolute angular momentum is quantized with $m\hbar$. [1]

Electrons in motion in a ring make up an electrical current flow. In the ground state of the system, electrons with positive and negative velocities v are evenly balanced, as long as there is an odd number of electrons. If we increase the magnetic flux and create an electron-hole pair, they still move in opposite directions. [2] The current for an electron moving in a positive direction is negative. We have to consider, that the mass of the hole is exactly negative of an electron mass $m_h = -m_e$. With positive charge and positive angular momentum, the current created by the hole is also negative. Overall it results to

$$I = -\frac{eL_e}{2\pi m_e R^2} - \frac{eL_h}{2\pi m_e R^2} = -\frac{em\hbar}{2\pi m_e R^2}. \tag{4.4}$$

The current in the ring induces a secondary magnetic field. This magnetic field has the reverse direction to the magnetic field inside the ring.

[1] In the separated-electrons picture we find that every electron gains the angular momentum of $1\hbar$. The total angular momentum is identical.

[2] The hole has a positive angular momentum $L = m_h vR$, but a negative mass.

Chapter 5

Conclusion

This thesis studied the excitations of electrons and electron-hole pairs in a ring. The fundamental phenomenon for our system was the Aharonov-Bohm effect. Electrons feel the influence of a magnetic flux inside the area in the ring, without being in contact with a magnetic field.

In Chapter 2 we examined static energy spectra over the magnetic flux Φ. The first ignored the δ potential in the Hamiltonian. It resulted in $E(n) = \frac{2\pi^2\hbar^2}{m_e C^2}(n - \frac{e}{2\pi c}\Phi)^2$. It has distinct energy states n, each can be occupied by one electron. For more than one electron a Fermi sea is formed. In this case, occupied states stay occupied even with changing magnetic flux.
The second spectrum included the δ potential. Energy bands with a band gap of $\Delta = \frac{\gamma}{\pi}$ formed. For small γ they were proportional to γ. In this case it is possible for electron states to change occupation status.

Chapter 3 approaches the system dynamically. The two cases from Chapter 2 are the border cases. The first represents the spectrum for rapid change of $A(t)$ or respectively the magnetic flux. The second case is the solution two the time independent Schrödinger equation. This allows us to examine the transition between these two scenarios. Everywhere where in case 1 a crossing of two electron states is, there is a energy gap in case 2. We found we can determine the probability of an electron tunneling through the Landau-Zener formula. For electrons near the Fermi energy this probability is $P_{LZ} = e^{-\frac{\gamma^2}{4\pi m v}}$. It is higher for a more rapid change of $A(t)$ and more electrons in the system.

We took the previous results and expressed them in the electron-hole picture in Chapter 4. Electron states in lower energies of the Fermi sea were never not occupied. Measurably, only the changes near the Fermi energy with changing magnetic flux are relevant. Therefore we described an electron-hole pair that is created through change of the magnetic flux.
The electron and hole have the properties of particle slightly above/under the Fermi energy. In a ring accelerated charged particles create a current $I = -\frac{em\hbar}{2\pi m_e R^2}$. This current is proportional to the total number of electrons in the system.

Overall, we found that electron excitations can be expressed through creation of electron-hole pair. If this electron-hole pair is spatially separated, at some point it would appear as if an only electron is created. Further studies in that direction lead to the phenomenon of the Chiral anomaly.

Appendix A

Gauge-Transformations

We want to solve the time independent Schrödinger equation for a Hamiltonian that includes the electromagnetic potential $A(x)$. We can transform

$$A(x) \to A' = A(x) + \partial_x \chi(x), \tag{A.1}$$

where A' is constant along x. Normally for a vector field we would use $\nabla\chi(x)$, but in this case we are only interested in A along x and only use the derivative in x instead. The Schrödinger equation transforms as well

$$H\Psi(x,t) = i\partial_t \Psi(x,t) \to H'\Psi'(x,t) = i\partial_t \Psi'(x,t). \tag{A.2}$$

into

$$\frac{1}{2m_e}\left[-i\hbar\partial_x + \frac{e}{c}A'\right]^2 \Psi'(x) = E\Psi'(x), \tag{A.3}$$

an equation we can solve easily. We want to find the operation on Ψ', that gives us the solution Ψ for the original Schrödinger equation. We start with putting $A' = A(x) + \chi(x)$ into the equation (A.3) and receive

$$\begin{aligned}
&-\hbar^2\partial_x^2\Psi'(x) - 2\frac{ie\hbar}{c}[A(x) + (\partial_x\chi(x))](\partial_x\Psi'(x)) \\
&-\frac{ie\hbar}{c}[\partial_x A(x) + (\partial_x^2\chi(x))]\Psi'(x) + \frac{e^2}{c^2}[A^2(x) + 2A(x)(\partial_x\chi(x)) + (\partial_x\chi(x))^2]\Psi'(x) \\
=&2m_e E\Psi'(x).
\end{aligned} \tag{A.4}$$

We express Ψ' as product of Ψ and a factor $c(x)$. That gives us:

$$\begin{aligned}
&\Psi'(x) = c(x)\Psi(x) \\
&\partial_x\Psi'(x) = (\partial_x c(x))\Psi(x) + c(x)(\partial_x\Psi(x)) \\
&\partial_x^2\Psi'(x) = (\partial_x c(x))\Psi(x) + 2(\partial_x c(x))(\partial_x\Psi(x)) + c(x)(\partial_x^2\Psi(x)).
\end{aligned} \tag{A.5}$$

Since we know Ψ', $c(x)$ is what we need to solve to calculate Ψ. We insert (A.5) into (A.4). We take the part

$$\begin{aligned}
&c(x)\left[-\hbar^2\partial_x\Psi(x) - \frac{i2e\hbar}{c}A(x)(\partial_x\Psi(x)) - \frac{ie\hbar}{c}(\partial_x A(x))\Psi(x) + \frac{e^2}{c^2}A(x)^2\Psi(x)\right] \\
=&c(x)\left[2m_e E\Psi(x)\right]
\end{aligned} \tag{A.6}$$

from both sides of the equation. The square brackets are the original Schrödinger equation $H\Psi = E\Psi$. They are definitively equal and can be removed. On both sides of the equation remains

$$\begin{aligned}
&\Psi(x)\Big[-\hbar^2\partial_x^2 c(x) - \frac{i2e\hbar}{c}(A(x)\partial_x c(x) + (\partial_x\chi(x))(\partial_x c(x))) \\
&- \frac{ie\hbar}{c}(\partial_x^2\chi(x))c(x) + \frac{e^2}{c^2}(2A(x)\partial_x\chi(x) + (\partial_x\chi(x))^2)c(x)\Big] \\
&+ (\partial_x\Psi(x))\left[-2\hbar^2\partial_x c(x) - \frac{i2e\hbar}{c}(\partial_x\chi(x))c(x)\right] = 0. \qquad \text{(A.7)}
\end{aligned}$$

We do not need a specific solution for $c(x)$, any will work. The easiest approach is to make both square brackets constantly 0. In that case we do not have any special limitations for Ψ. We start with the second bracket, that gives us the condition

$$-2\hbar^2\partial_x c(x) - \frac{i2e\hbar}{c}(\partial_x\chi(x))c(x) = 0. \qquad \text{(A.8)}$$

It results in the factor

$$c(x) = ae^{-\frac{ie}{c\hbar}\chi(x)} \qquad \text{(A.9)}$$

with a an arbitrary constant, we ignore. This solution also fulfills the condition, that the first square bracket from (A.7) equals to 0. We go back to (A.5) and know

$$\Psi(x) = e^{\frac{ie}{c\hbar}\chi(x)}\Psi'(x). \qquad \text{(A.10)}$$

Appendix B

Conservation of canonical angular momentum

We have a system of an electron in a ring, with no additional potentials. We write $\psi = \frac{2\pi}{C}x$, the angular rotation:

$$\begin{aligned} x_1 &= R\cos\psi \\ x_2 &= R\sin\psi \end{aligned} \tag{B.1}$$

The radius R is fixed. Inside the ring there is a magnetic field with an constant electromagnetic potential A along the ring. The Lagrangian is

$$\mathcal{L} = \frac{m_e R^2 \dot{\psi}^2}{2} - \frac{e}{c}R\dot{\psi}A \tag{B.2}$$

with the negative charge $q = -e < 0$. Since ψ is the canonical coordinate, the canonical momentum is

$$P_\psi = \partial_{\dot{\psi}}\mathcal{L} = m_e R^2\dot{\psi} - \frac{e}{c}RA \tag{B.3}$$

the angular momentum. We can rearrange (B.3) into the angular velocity

$$\dot{\psi} = \frac{1}{m_e R^2}(P_\psi + \frac{e}{c}AR). \tag{B.4}$$

Together with the canonical momentum and the Lagrangian we find the Hamiltonian

$$\begin{aligned} H = P_\psi\dot{\psi} - \mathcal{L} &= \frac{P_\psi^2}{2m_e R^2} + \frac{P_\psi \frac{e}{c}AR}{m_e R^2} + \frac{\frac{e^2}{c^2}A^2R^2}{2m_e R^2} \\ &= \frac{1}{2m_e R^2}(P_\psi + \frac{e}{c}AR)^2 \end{aligned} \tag{B.5}$$

as known from (2.1).

There is a rotational symmetry in ψ. The Noether theorem states, that for every symmetry in a system, there is a conserved quantity. The Lagrangian is invariant to the transformation $\psi \to \psi(t,\alpha) = \phi(t,0) + \alpha(t)$ of the angular momentum. That means:

$$
\begin{aligned}
\left.\frac{d\mathcal{L}}{d\alpha}\right|_{\alpha=0} &\stackrel{!}{=} 0 \\
&= \left.\frac{\partial\mathcal{L}}{\partial\psi}\frac{\partial\psi}{\partial\alpha} + \frac{\partial\mathcal{L}}{\partial\dot{\psi}}\frac{\partial\dot{\psi}}{\partial\alpha}\right|_{\alpha=0} \\
&= \left.\frac{\partial\mathcal{L}}{\partial\psi}\frac{\partial\psi}{\partial\alpha} + \frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{\psi}}\frac{\partial\psi}{\partial\alpha}\right) - \left(\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{\psi}}\right)\frac{\partial\psi}{\partial\alpha}\right|_{\alpha=0}.
\end{aligned}
\tag{B.6}
$$

In the last line we used $\frac{\partial\mathcal{L}}{\partial\dot{\psi}}\frac{\partial\dot{\psi}}{\partial\alpha} = \frac{\partial\mathcal{L}}{\partial\dot{\psi}}\left(\frac{d}{dt}\frac{\partial\psi}{\partial\alpha}\right)$. This can be transformed into the term above using the product rule. We use the Euler-Lagrange formula $\frac{\partial\mathcal{L}}{\partial\psi} - \frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{\psi}} = 0$ to eliminate the first and third term. What remains is

$$
\left.\frac{d\mathcal{L}}{d\alpha}\right|_{\alpha=0} = \left.\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{\psi}}\frac{\partial\psi}{\partial\alpha}\right)\right|_{\alpha=0}.
\tag{B.7}
$$

Therefore, we can conclude that $\frac{\partial\mathcal{L}}{\partial\dot{\psi}}\frac{\partial\psi}{\partial\alpha} = \text{const}$. The derivative of α for the angular rotation is $\partial_\alpha\psi = 1$. The canonical angular momentum $P_\psi = \partial_{\dot{\psi}}\mathcal{L}$ is conserved.

Appendix C

Nearly degenerate perturbation theory

We start with a Hamiltonian $H^{(0)}$ of which we know the solution and a perturbation $H^{(1)}$.

$$H = H^{(0)} + H^{(1)} \tag{C.1}$$

Perturbation theory analyses an unknown Hamiltonian with knowledge about a similar Hamiltonian. For a small perturbation we expect similar behavior. Specifically we expect the eigenstates and eigenvalues to be a power series of γ. The first element

$$\frac{v_1}{E_n - E_m} \tag{C.2}$$

diverges for $E_n \to E_m$. In the degenerate case the energies are the same, in the nearly degenerate case the difference is very small. Therefore, v_1 has to be small as well.
We can write the Hamiltonian matrix as such

$$H = \begin{pmatrix} E_n + v_0 & v_1^* \\ v_1 & E_m + v_0 \end{pmatrix} \tag{C.3}$$

The eigenvalues of this matrix are

$$E_\pm = v_0 + \frac{E_n + E_m}{2} \pm \sqrt{\left(\frac{E_n - E_m}{2}\right)^2 + v_1^2}. \tag{C.4}$$

We develop these for $E_n - E_m >> v_1$ in 1. order:

$$\begin{aligned} E_+ &= E_n + v_0 \\ E_- &= E_m + v_0. \end{aligned} \tag{C.5}$$

These are the diagonal matrix elements.
When we look at band gaps, the energies in $H^{(0)}$ used to be degenerate in crossings. The difference $E_n - E_m << v_1$ is still small. With an energy of $E_\pm \to E_{n,m} \pm v_1$ we find an energy gap of $2v_1$.

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Appendix D

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