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Numerical Investigation of the Upper Critical Field of a BCS - Superconductor

Semesterthesis

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Abstract

The goal of this semester project was to numerically investigate the determination of the upper critical field H_{c2} for a two-dimensional tight-binding model on a square lattice with on-site pairing. For that we have considered two couplings to the magnetic field, Zeeman coupling and coupling to the electrons orbital motion via Peierls substitution.

We have studied the Bogoliubov de Gennes approach which enables to consider systems with open boundary conditions and investigated it numerically.

As it turns out, we did not consider the full physical picture since below the critical temperature we also encounter the screening of the magnetic field (Meissner effect) which is rather complicated to treat. Therefore, the results for the upper critical field curve $H_{c2}(T)$ do not describe the correct physics. We however obtained values for the critical temperature but we did not manage to verify/compare them with the solutions of the linearized gap equation since its numerical implementation was unstable.

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1 Introduction

The process of interacting electrons of a material with an external magnetic field may destroy the superconducting state of that material. Such a coupling can happen through the electrons' spin, i.e., Zeeman coupling or through the electrons' orbital motion. The latter one can be realized through the Peierls substitution for tightly-bound electrons.

The question that now arises is, for which configurations of temperature and magnetic field does the superconducting phase of a material vanish? The upper critical field H_{c2} of a superconductor is of great importance for applications like superconducting magnets in magnetic resonance imaging or nuclear magnetic resonance.

From a theoretical perspective, H_{c2} provides essential insights into the properties of superconductors. The magnitude and transition line of H_{c2} offer valuable information about the superconducting order parameter as well as the coherence length and penetration depth, which are fundamental for the understanding of the microscopic behavior of a superconductor.

In this project we investigate the magnetic response of a tight binding model on a square lattice by adding different magnetic interaction terms. Combining analytical and numerical approaches we derive the self consistency equation which is then solved numerically for the order parameter and therefore for the critical temperature T_C and critical field H_{c2} .

2 Theory

For our study we consider a 2-dimensional square lattice and assume that the electrons of our system are tightly bound. Hence our system is described by a tight binding Hamiltonian.

$$\hat{H} = \hat{H}_0 + \hat{H}' = - \sum_{\langle i,j \rangle} t_{ij} \hat{c}_i^\dagger \hat{c}_j + \text{h.c.} + \sum_{i,j,k,l} V_{ijkl} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i, \quad (1)$$

where we have omitted the spin indices for brevity. The last term in the above Hamiltonian accounts for the chemical potential μ . For the further analysis we usually go to reciprocal space, so we partially or fully conduct a Fourier transform on our Hamiltonian depending on the type of boundary conditions.

Next let us discuss how the magnetic field can interact with the electrons of our system. There are essentially two ways how a coupling can happen, namely through the electron's spin or in the orbital motion. We choose our coordinate system such that the lattice lays in the xy-plane and assume that the magnetic field points perpendicular into z-direction. In the following two subsections we discuss how the magnetic field changes the Hamiltonian of our system (1). The detailed derivations of transforming the Hamiltonian into Fourier space can be found in the appendix.

2.1 Zeeman Coupling

The spins of the electrons can couple to the magnetic field \vec{B} via Zeeman coupling

$$-\mu \vec{B} \cdot \vec{S}, \quad (2)$$

where \vec{S} is the spin operator and in the case of spin- $\frac{1}{2}$ it holds that $\vec{S} = \frac{1}{2} \vec{\sigma} = \frac{1}{2} (\sigma^x, \sigma^y, \sigma^z)$, where σ^i are the Pauli matrices.

To simplify the expression we assume the magnetic field to be constant and aligned along the z-axis. Thus our tight-binding Hamiltonian with Zeeman coupling, Fourier transformed in y-direction, is

given by

$$\begin{aligned}\hat{H} = & \frac{-t}{2} \sum_{i_x, k_y, \sigma} \left(\hat{c}_{i_x, k_y, \sigma}^\dagger \hat{c}_{i_x+1, k_y, \sigma} + \hat{c}_{i_x, k_y, \sigma}^\dagger \hat{c}_{i_x-1, k_y, \sigma} + \text{h.c.} \right) + 4 \cdot \cos(k_y a_y) \hat{c}_{i_x, k_y, \sigma}^\dagger \hat{c}_{i_x, k_y, \sigma} \\ & - \frac{B}{2} \sum_{i_x, k_y} \left(\hat{c}_{i_x, k_y, \uparrow}^\dagger \hat{c}_{i_x, k_y, \uparrow} - \hat{c}_{i_x, k_y, \downarrow}^\dagger \hat{c}_{i_x, k_y, \downarrow} \right) - \mu \sum_{i_x, k_y, \sigma} \hat{c}_{i_x, k_y, \sigma}^\dagger \hat{c}_{i_x, k_y, \sigma}.\end{aligned}\quad (3)$$

In the latter we denote by a_y the lattice constant in y-direction.

2.2 Peierls Substitution

So far we have assumed that the coupling constant $t_{ij} = t$ is constant in the tight binding model (1). We now consider the case where the magnetic field interacts with the electrons through their orbital motion:

$$t_{ij} \rightarrow t_{ij} \cdot e^{i \frac{e}{\hbar} \int_i^j \vec{A} \cdot d\vec{r}} \quad (4)$$

This is the so called Peierls substitution. In the following discussion we set $\hbar = 1$.

The Hamiltonian that we derive hereinafter is also referred to as the Hofstadter model.

We fix the gauge freedom by choosing the field to be in the Landau gauge, i.e. $\vec{A} = (0, Bx, 0)$. As a first step we assume to have periodic boundary conditions. Then, the hopping in x- respectively y-direction takes the form

$$\begin{aligned}\vec{r} \rightarrow \vec{r} + \vec{e}_x : \int_{\vec{r}}^{\vec{r} + \vec{e}_x} \vec{A} \cdot d\vec{r} &= B \int_{\vec{r}}^{\vec{r} + \vec{e}_x} x \vec{e}_y \cdot \vec{e}_y = 0, \\ \vec{r} \rightarrow \vec{r} + \vec{e}_y : \int_{\vec{r}}^{\vec{r} + \vec{e}_y} \vec{A} \cdot d\vec{r} &= B \int_{\vec{r}}^{\vec{r} + \vec{e}_y} x \vec{e}_y \cdot \vec{e}_y = Ba_y x, \\ \implies e^{ie \int \vec{A} \cdot d\vec{r}} \hat{c}_{\vec{r} + \vec{e}_y}^\dagger \hat{c}_{\vec{r}} &= e^{ieBa_y x} \hat{c}_{\vec{r} + \vec{e}_y}^\dagger \hat{c}_{\vec{r}} = e^{ie\phi x/a_x} \hat{c}_{\vec{r} + \vec{e}_y}^\dagger \hat{c}_{\vec{r}}\end{aligned}\quad (5)$$

with $\phi = Ba_x a_y$ the magnetic flux through the unit cell with area $a_x a_y$. Hence our Hamiltonian looks like

$$\hat{H} = - \sum_{\vec{r}} t \hat{c}_{\vec{r} + \vec{e}_x}^\dagger \hat{c}_{\vec{r}} + t e^{i\phi x} \hat{c}_{\vec{r} + \vec{e}_y}^\dagger \hat{c}_{\vec{r}} + \text{h.c.} \quad (6)$$

where we have set $a_x = a_y = 1, e = 1$ and $x \in \mathbb{N}$. Since ϕ is part of phase factor we know that it is 2π periodic thus we can restrict to $\phi \in [0, 2\pi]$.

We notice that the Hamiltonian (6) is still y-translation invariant but the phase breaks translation symmetry in x-direction.

Periodic boundary conditions along x impose that

$$e^{i\phi x} \Big|_{x=N_x} = e^{i\phi x} \Big|_{x=0}, \quad (7)$$

where N_x is the size of the system. Therefore

$$\phi N_x = 2\pi n \Rightarrow \phi = \frac{2\pi n}{N_x}, n \in \mathbb{N}. \quad (8)$$

Thus the general form of the magnetic flux is

$$\phi = \frac{2\pi s}{q}, \text{ where } s, q \text{ are coprime integers.} \quad (9)$$

If the magnetic flux takes on specific values corresponding to a coprime ratio as above, the periodicity of the Hamiltonian is restored, but the unit cell is expanded by a factor of q . In other words we can perform the Fourier transformation in all dimensions.

On the other hand if we assume open boundary conditions in x -direction, the Hamiltonian (6) cannot be Fourier transformed completely due to the phase. However we can block diagonalize the Hamiltonian by performing the Fourier transform only in y -direction and we obtain

$$\hat{H} = -t \cdot \sum_{i,k} \left(\hat{c}_{x_i+1,k}^\dagger \hat{c}_{x_i,k} + \text{h.c.} \right) + [2 \cos(k - \phi x_i) - \mu] \hat{c}_{x_i,k}^\dagger \hat{c}_{x_i,k} \quad (10)$$

where $x_i = 0, 1, \dots, N_x$ are the positions of the lattice in x -direction. k are the y -components of the reciprocal vectors of the first Brillouin zone. The detailed calculation can be found in the appendix A.3.

2.2.1 Landau Levels

For small magnetic fluxes $\phi \ll 1$ we should recover the Landau levels $E_n = \hbar\omega_c (n + \frac{1}{2})$ [1].

We quickly derive this relation. First we want to determine an expression for the effective mass m^* for the present band structure by expanding the tight binding dispersion for $B = 0$

$$\epsilon_{\vec{k}} = -2t \left(\cos(\vec{k} \cdot \vec{a}_x) + \cos(\vec{k} \cdot \vec{a}_y) \right) = -4t + ta^2 \vec{k}^2 + \mathcal{O}(\vec{k}^3), \quad (11)$$

where we have assumed that $|\vec{a}_x| = |\vec{a}_y| = a$. Comparing the quadratic term with $\hbar^2 \vec{k}^2 / 2m^*$ we obtain

$$m^* = \frac{\hbar^2}{2ta^2}.$$

Since the magnetic field is the flux per unit area, i.e., $B = \hbar c \phi / ea^2$ we can rewrite the cyclotron frequency ω_c as

$$\omega_c = \frac{eB}{m^*} = \frac{\hbar e}{c} \cdot \frac{\hbar c \phi}{ea^2} \cdot \frac{2ta^2}{\hbar^2} = 2\phi t. \quad (12)$$

Thus the Landau spectrum (for $\phi \ll 1$) is given by

$$E_n(\phi) = 2\phi t \left(n + \frac{1}{2} \right), \quad n \in \mathbb{N}. \quad (13)$$

We will verify them by plotting the energy spectrum of the Hofstadter Hamiltonian for small flux values, see fig. 9.

2.3 BCS Theory

So far we have introduced how the Hamiltonian of our system changes with different magnetic couplings. We have seen that for certain couplings we destroy the periodic boundaries which means the Hamiltonian is not Fourier transformable in all directions. Therefore we need another approach than mean field theory in order to obtain a self consistency equation for the order parameter Δ . Nonetheless let us briefly review the self consistency equation in the BCS case. We start from the BCS Hamiltonian of the form [2]

$$\hat{H}_{BCS} = \sum_{\vec{k},s} \underbrace{(\epsilon_{\vec{k}} - \mu)}_{\xi_{\vec{k}}} \hat{c}_{\vec{k},s}^\dagger \hat{c}_{\vec{k},s} + \sum_{\vec{k},\vec{k}'} V_{\vec{k},\vec{k}'} \hat{c}_{\vec{k}\uparrow}^\dagger \hat{c}_{-\vec{k}\downarrow}^\dagger \hat{c}_{-\vec{k}'\downarrow} \hat{c}_{\vec{k}'\uparrow}. \quad (14)$$

Assuming an uniform interaction $V_{\vec{k}, \vec{k}'} = V$ and performing a mean field approach we arrive at the self consistency equation [2]

$$\Delta = -\frac{V}{N} \sum_{\vec{k} \in 1. \text{ BZ}} \frac{\Delta}{2E_{\vec{k}}} \tanh\left(\frac{\beta E_{\vec{k}}}{2}\right) \quad (15)$$

where $E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + \Delta^2}$ and N is the number of unit cells.

We use the solutions of this self consistency equation for an s-wave superconductor in order to get a good initial value for the generalized case later. As a next step we discuss how to derive a self consistency equation in the case of open boundaries.

2.4 Bogoliubov-de-Gennes Method

Our starting point is a generic tight binding Hamiltonian with pairing terms

$$\hat{H} = \sum_{i,j,\sigma} \hat{c}_{i\sigma}^\dagger h_{ij} \hat{c}_{j\sigma} + \sum_{ij} \Delta_{i\uparrow j\downarrow} \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger + \Delta_{i\uparrow j\downarrow}^* \hat{c}_{i\downarrow} \hat{c}_{j\uparrow}. \quad (16)$$

Assuming singlet pairing, we define

$$\Delta_{i\uparrow j\downarrow} = \frac{V}{2} (\langle c_{j\downarrow} c_{i\uparrow} \rangle - \langle c_{j\uparrow} c_{i\downarrow} \rangle). \quad (17)$$

By rephrasing terms $c_{i\sigma}^\dagger c_{j\sigma} = \frac{1}{2} (c_{i\sigma}^\dagger c_{j\sigma} - c_{j\sigma} c_{i\sigma}^\dagger)$, the same for $c^\dagger c^\dagger$ and cc terms, we can rewrite the Hamiltonian (16) as

$$\hat{H} = \frac{1}{2} \vec{c}^\dagger \begin{pmatrix} h_{\uparrow\uparrow} & 0 & 0 & \hat{\Delta} \\ 0 & h_{\downarrow\downarrow} & -\hat{\Delta}^T & 0 \\ 0 & -\hat{\Delta}^* & -h_{\uparrow\uparrow}^* & 0 \\ \hat{\Delta}^\dagger & 0 & 0 & -h_{\downarrow\downarrow}^* \end{pmatrix} \vec{c} = \frac{1}{2} \vec{c}^\dagger H \vec{c} \quad (18)$$

where we have defined $\vec{c} = (c_{1\uparrow}, \dots, c_{m\uparrow}, c_{1\downarrow}, \dots, c_{m\downarrow}, c_{1\uparrow}^\dagger, \dots, c_{m\downarrow}^\dagger)$.

We are now looking for vectors \vec{w} of the form $(u_{1\uparrow}, \dots, u_{m\uparrow}, u_{1\downarrow}, \dots, u_{m\downarrow}, v_{1\uparrow}, \dots, v_{m\uparrow}, v_{1\downarrow}, \dots, v_{m\downarrow}) = (\vec{u}, \vec{v})$, such that they fulfill the properties of being an eigenvector of the single particle Hamiltonian H ,

$$H \begin{pmatrix} \vec{u}_n \\ \vec{v}_n \end{pmatrix} = E_n \begin{pmatrix} \vec{u}_n \\ \vec{v}_n \end{pmatrix}. \quad (19)$$

Let us denote the complex conjugation by the operator \hat{K} and define $S_x = \sigma_x \otimes \mathbf{1}_{2 \times 2}$. It is then easy to check that the following relation holds for H ,

$$S_x \hat{K} H \hat{K} S_x = \begin{pmatrix} 0 & \mathbf{1}_{2 \times 2} \\ \mathbf{1}_{2 \times 2} & 0 \end{pmatrix} \hat{K} H \hat{K} \begin{pmatrix} 0 & \mathbf{1}_{2 \times 2} \\ \mathbf{1}_{2 \times 2} & 0 \end{pmatrix} = -H. \quad (20)$$

This is nothing but the particle-hole symmetry of the redundant BdG-Hamiltonian H . This implies if \vec{w}_n is an eigenvector of H with eigenvalue E_n , $S_x \hat{K} \vec{w}_n$ is an eigenstate of H with eigenenergy $-E_n$.

Now the $\langle cc \rangle$ expressions in equation (17) can be expressed through the anomalous Greens function

$$\langle c_{j\downarrow} c_{i\uparrow} \rangle = F_{j\downarrow i\uparrow}(\tau = 0) = -\frac{1}{\beta} \sum_{n,\omega} \frac{\vec{u}_{j\downarrow}^n \vec{v}_{i\uparrow}^{*n}}{i\omega - E_n}. \quad (21)$$

The sum above runs over all fermionic Matsubara frequencies ω and all eigen-energies of H . The fermionic Matsubara frequencies are defined as $\omega_n = \frac{(2n+1)\pi}{\beta}$, $n \in \mathbb{Z}$. We can now perform the Matsubara summation ¹, i.e.,

$$\frac{1}{\beta} \sum_{\omega} \frac{1}{i\omega - E} = n_F(E) = \frac{1}{2} (1 - \tanh(\beta E/2)), \quad (22)$$

and we obtain the self consistency equation in 1d

$$\Delta_{i\uparrow j\downarrow} = \frac{V}{2} (\langle c_{j\downarrow} c_{i\uparrow} \rangle - \langle c_{j\uparrow} c_{i\downarrow} \rangle) = -\frac{V}{4} \sum_n (\bar{u}_{j\downarrow}^n \bar{v}_{i\uparrow}^{*n} + \bar{v}_{j\downarrow}^n \bar{u}_{i\uparrow}^{*n}) \tanh\left(\frac{\beta E_n}{2}\right). \quad (23)$$

In the case of on site pairing, i.e., $i = j$, the above equation reduces to

$$\Delta_{i\uparrow i\downarrow} = -\frac{V}{2} \sum_n \bar{u}_{i\downarrow}^n \bar{v}_{i\uparrow}^{*n} \tanh\left(\frac{\beta E_n}{2}\right). \quad (24)$$

Now we consider a two dimensional system, with only onsite interaction, periodic boundaries in y-direction and open boundary conditions in x-direction. The singlet order parameter is then given by

$$\Delta_x = \frac{V}{N_y} \sum_{k_y} (\langle c_{x,k_y,\downarrow} c_{x,-k_y,\uparrow} \rangle - \langle c_{x,k_y,\uparrow} c_{x,-k_y,\downarrow} \rangle). \quad (25)$$

Hence the Hamiltonian (18) is slightly modified to

$$\hat{H} = \frac{1}{2} \sum_{k_y} \vec{c}_{k_y}^\dagger H(k_y) \vec{c}_{k_y}, \quad (26)$$

where the vector \vec{c}_{k_y} is given by

$$\vec{c}_{k_y} = \left(c_{k_y,1,\uparrow}, \dots, c_{k_y,N_x,\uparrow}, c_{k_y,1,\downarrow}, \dots, c_{k_y,N_x,\downarrow}, c_{-k_y,1,\uparrow}^\dagger, \dots, c_{-k_y,N_x,\downarrow}^\dagger \right). \quad (27)$$

Each block $h_{\sigma\sigma} \rightarrow h_{\sigma\sigma}(k_y)$ is now a matrix in x-position space of size $N_x \times N_x$. We again are looking for eigenvectors $\vec{w}_{k_y} = (\bar{u}_{k_y}, \bar{v}_{k_y})$ such that

$$\begin{pmatrix} h_{\uparrow\uparrow}(k_y) & 0 & 0 & \hat{\Delta} \\ 0 & h_{\downarrow\downarrow}(k_y) & -\hat{\Delta}^T & 0 \\ 0 & -\hat{\Delta}^* & -h_{\uparrow\uparrow}^*(-k_y) & 0 \\ \hat{\Delta}^\dagger & 0 & 0 & -h_{\downarrow\downarrow}^*(-k_y) \end{pmatrix} \begin{pmatrix} \bar{u}_{k_y,\uparrow}^n \\ \bar{u}_{k_y,\downarrow}^n \\ \bar{v}_{k_y,\uparrow}^n \\ \bar{v}_{k_y,\downarrow}^n \end{pmatrix} = E_n \begin{pmatrix} \bar{u}_{k_y,\uparrow}^n \\ \bar{u}_{k_y,\downarrow}^n \\ \bar{v}_{k_y,\uparrow}^n \\ \bar{v}_{k_y,\downarrow}^n \end{pmatrix}. \quad (28)$$

We again recover the particle-hole symmetry for the blocks $H(k_y)$ from equation (26) slightly modified to

$$S_x \hat{K} H(k_y) \hat{K} S_x = -H(-k_y). \quad (29)$$

Hence $S_x \hat{K} (\bar{u}_{k_y,\uparrow}^n, \bar{u}_{k_y,\downarrow}^n, \bar{v}_{k_y,\uparrow}^n, \bar{v}_{k_y,\downarrow}^n)^T = (\bar{v}_{k_y,\uparrow}^{*n}, \bar{v}_{k_y,\downarrow}^{*n}, \bar{u}_{k_y,\uparrow}^{*n}, \bar{u}_{k_y,\downarrow}^{*n})^T$ is an eigenvector of $H(-k_y)$ with eigenvalue $-E_n$.

By expanding the order parameter (25) in terms of the Matsubara frequencies and eigenvectors of

¹The most used summations can be found here: https://en.wikipedia.org/wiki/Matsubara_frequency

$H(k_y)$ and performing the Matsubara summation, we obtain the self consistency equation for the order parameter

$$\begin{aligned}\Delta_x &= \frac{V}{2N_y} \sum_{\omega, k_y, n} \frac{\vec{u}_{x,\downarrow}^n(k_y) \vec{v}_{x,\uparrow}^{n*}(k_y)}{i\omega - E_n(k_y)} - \frac{\vec{u}_{x,\uparrow}^n(-k_y) \vec{v}_{x,\downarrow}^{n*}(-k_y)}{i\omega - E_n(-k_y)} \\ &= \frac{V}{2N_y} \sum_{\omega, k_y, n} \frac{\vec{u}_{x,\downarrow}^n(k_y) \vec{v}_{x,\uparrow}^{n*}(k_y)}{i\omega - E_n(k_y)} - \frac{\vec{v}_{x,\uparrow}^{n*}(k_y) \vec{u}_{x,\downarrow}^n(k_y)}{i\omega + E_n(k_y)} \\ &= -\frac{V}{2N_y} \sum_{m, k_y} u_{x,\downarrow}^m(k_y) v_{x,\uparrow}^{*m}(k_y) \tanh\left(\frac{\beta E_m(k_y)}{2}\right).\end{aligned}\quad (30)$$

To go from the first to second line we exactly used the aforementioned particle-hole symmetry. Note that Δ_x is a vector of length N_x , i.e., the size in x-direction.

2.5 Numerical Calculations

For our numerical tasks we lay our focus on equations (24) and (30). The equations can be used to compute numerically the order parameter for an arbitrary non-interacting Hamiltonian at given temperature T and magnetic field H .

The goal is to determine the critical field $H_{c2}(T)$ of such a Hamiltonian, i.e., at a given temperature we are looking for the highest possible magnetic field, such that a solution to the self-consistency equations still exists. We try two attempts to determine the critical field

1. rewrite the self consistency equation as a root problem and solve them with the `scipy.optimize.root` and `scipy.optimize.fsolve` by brute force
2. solve the equation recursively until the order parameter converges with a certain tolerance.

In both cases we need an initial guess to start the iterative solving. We usually choose the order parameter of the mean field equation (15).

In order to determine the critical field, we solve the self consistency equation with the above mentioned methods at given temperature and magnetic field strength and perform a sweep over temperature and magnetic field.

2.6 Gorkov Equations (Outlook)

We can derive a linearized gap equation from the Gor'kov equations which enables us to determine the transition temperature T_C in the presence of a magnetic field. Following the steps in Mineev's book [3], we expand the anomalous Green's function F in the order parameter Δ to first order since Δ is small around T_C . Additionally we assume only onsite coupling, which means that appearing spin indices have to be unequal due to Pauli's principle.

We end up with an eigenvector equation for the order parameter $\Delta_{\uparrow,\downarrow}^{xx}$

$$\begin{aligned}\Delta_{\uparrow,\downarrow}^{xx} &= \\ &= -\frac{V}{2N_y} \sum_{k_y} \sum_{q,p=1}^{N_x} \sum_l (\vec{v}_l(k_y) \cdot \vec{v}_l^\dagger(k_y))_{\uparrow,\uparrow}^{x,p} \Delta_{\uparrow,\downarrow}^{p,q} \sum_r (\vec{v}_r(k_y) \cdot \vec{v}_r^\dagger(k_y))_{\downarrow,\downarrow}^{x,q} \left[\frac{n_F(E_l(k_y)) - n_F(-E_r(-k_y))}{E_l(k_y) + E_r(k_y)} \right].\end{aligned}\quad (31)$$

Here the $\vec{v}_l(k_y)$ are the eigenvectors of the k_y - corresponding block of the normal state single particle Hamiltonian H_0 , i.e.

$$H_0(k_y)\vec{v}_l(k_y) = E_l(k_y)\vec{v}_l(k_y), \quad \vec{v}_l \in \mathbb{R}^{2N_x}. \quad (32)$$

In other words, at the transition point, the order parameter is an eigenvector of the above equation with eigenvalue 1. This approach is much more appealing since we have to diagonalize the normal state Hamiltonian once for a given magnetic field strength and can then perform the sweep over temperature. In contrast, the BdG approach is much more numerically demanding since we have to diagonalize a matrix in each iterative step in the solving procedure of the self-consistency equation for a given magnetic field and temperature.

3 Results

3.1 Order Parameter Temperature Dependence for Mean Field Problem

We first present in Figure 1 the temperature dependence of the order parameter in the case of the mean field Hamiltonian for different ratios of V/t . Regarding this ratio V/t , we always choose $t = 1$ for the whole investigation. We use the solutions of the mean field problem with periodic boundary

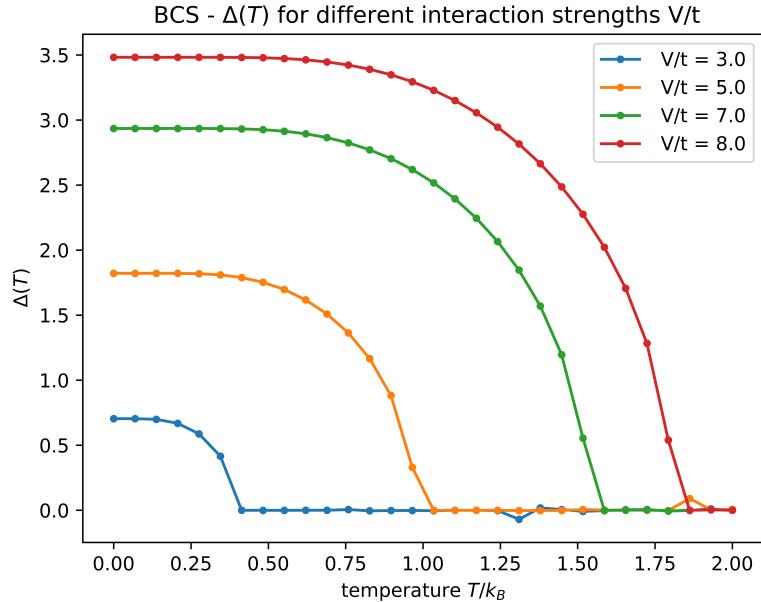


Figure 1: Plot of temperature dependence of the order parameter of the mean field problem. We assumed here a square lattice of size 100×100 . In order to solve equation (15) we use the `scipy.optimize.fsolve`.

conditions as a initial guess for the iterative computations in the BdG-formalism in the case of open boundary conditions.

3.2 Critical H-Field Analysis in One Dimension

Next we show the result of the critical magnetic field H_{c2} for a one dimensional chain where the magnetic field interacts with the system through Zeeman coupling (see Figure 2). To be more specific, we solve equation (24) recursively. Let us briefly discuss how the recursion works.

We begin by solving for the order parameter of the mean field problem, which is then used to construct the BdG Hamiltonian (18). After diagonalizing the resulting matrix, the corresponding eigenvalues and eigenvectors are used to update the (non-homogeneous) order parameter according to (24). This process is repeated iteratively until the order parameter converges.

To compute the critical field, we use the solution of the order parameter from the mean field problem as an initial guess, then progressively increase the magnetic field until the order parameter converges to zero.

In this situation we use on the one hand the root solver from the *scipy*-module and on the other hand an iterative solver to determine the critical field. The computation duration for the root solver takes almost twice as long as the iterative procedure which is already a large discrepancy for a rather small system size of 64. This indicates that the root solvers are not a convenient way to solve the self consistency equation.

This statement is reinforced when we try to solve the equation for a two dimensional system. In this case, the root solver even has problems with convergence.

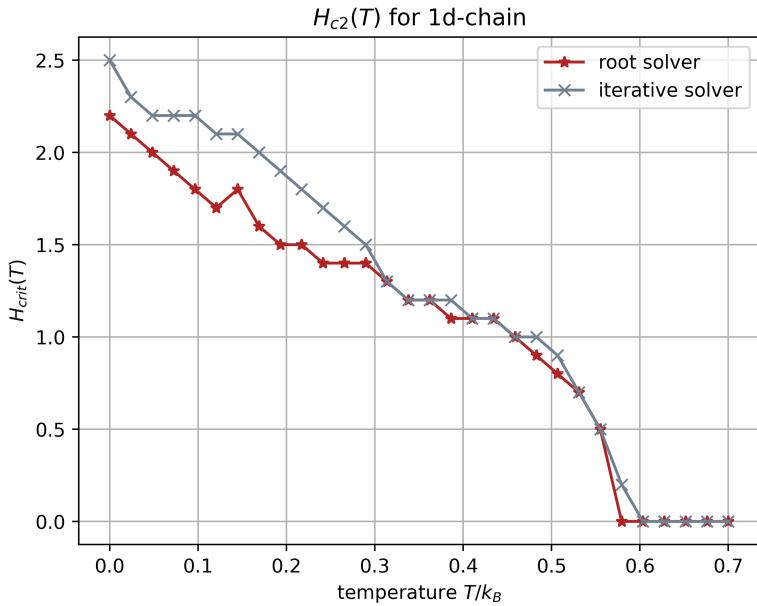
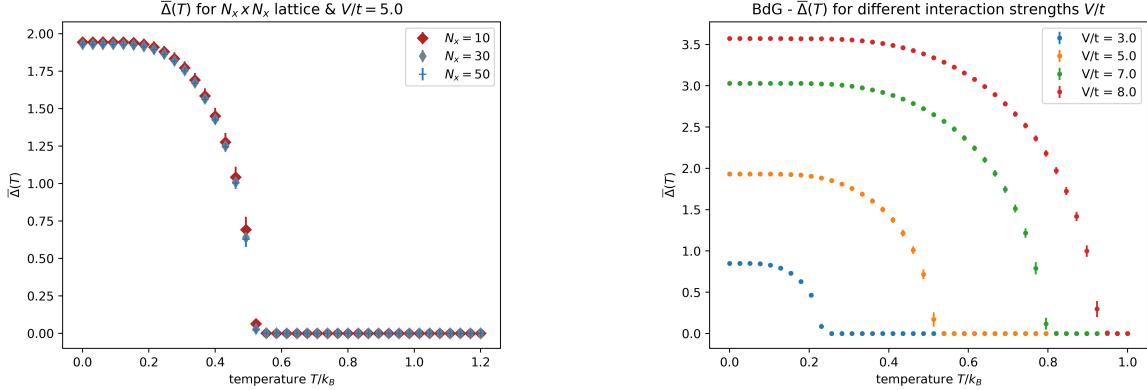


Figure 2: Calculation of the upper critical field for a 1d system with Zeeman coupling. The system size is 64 and we use the `scipy.optimize.root`-routine and an iterative procedure to solve the self consistency equation (24). The computation time is almost twice as long for the root solver.

3.3 Examination in Two Dimensions

We thus use an iterative solver for all the following computations. In Figure 3a we plot the temperature dependence of the order parameter $\bar{\Delta}$ (averaged over all lattice sites) for different sizes of square lattices. We observe that the critical temperatures respectively the curves coincide for the different sizes. In Figure 3b we plot the temperature dependence of the order parameter for different

interactions strengths V/t . In Figure 4 we plot the space dependence of the order parameter $\Delta(x_i)$ with respect to the lattice site x_i . We choose the number of lattice sites to be $N_x = 50$.



(a) Plot of $\bar{\Delta}$ as a function of temperature for different system sizes of a square lattice. Critical temperature is at $T_C = 0.53$ and is equal for all system sizes.

(b) Plot of $\bar{\Delta}$ as a function of temperature for a 30×30 square lattice for different ratios of V/t .

Figure 3: On the left we plot the temperature dependence of the order parameter $\Delta(T)$ for different lattice sizes. On the right we show $\Delta(T)$ for different interaction strengths V/t . One can directly read off the critical temperature T_C , i.e., the smallest temperature at which the order parameter vanishes.

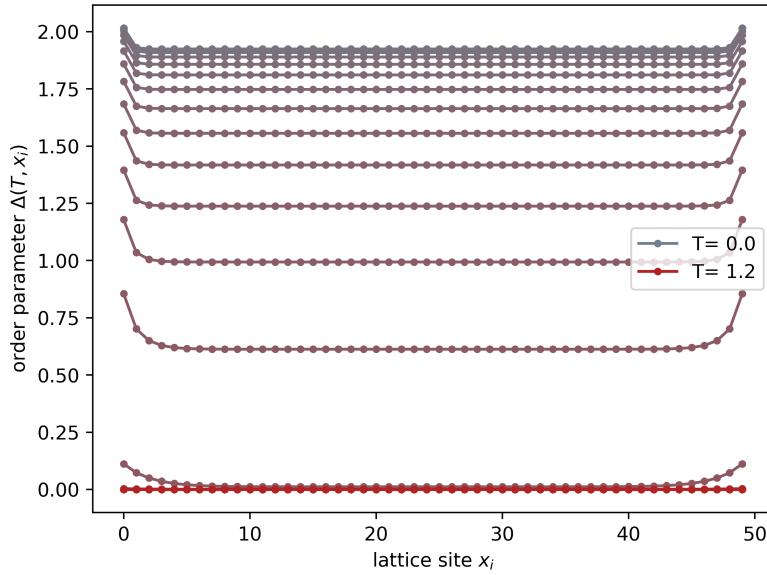


Figure 4: Order parameter $\Delta(T, x_i)$ as a function of lattice site $x_i = 1, \dots, N_x$. In our case $N_x = 50$. The temperature ranges from $T = 0.0$ (gray curves) until $T = 1.2$ (red curves). We observe that for $T = 1.2$ the order parameter Δ vanishes the first time at all lattice sites. Hence that is exactly the critical temperature.

3.3.1 Critical H-field Analysis for Zeeman Coupling

Next let us include an interaction with the magnetic field (again Zeeman coupling) and compute the upper critical field H_{c2} of a two dimensional square lattice for different configurations.

In Figure 5 we have computed the upper critical field for a 30×30 lattice for different interactions strengths.

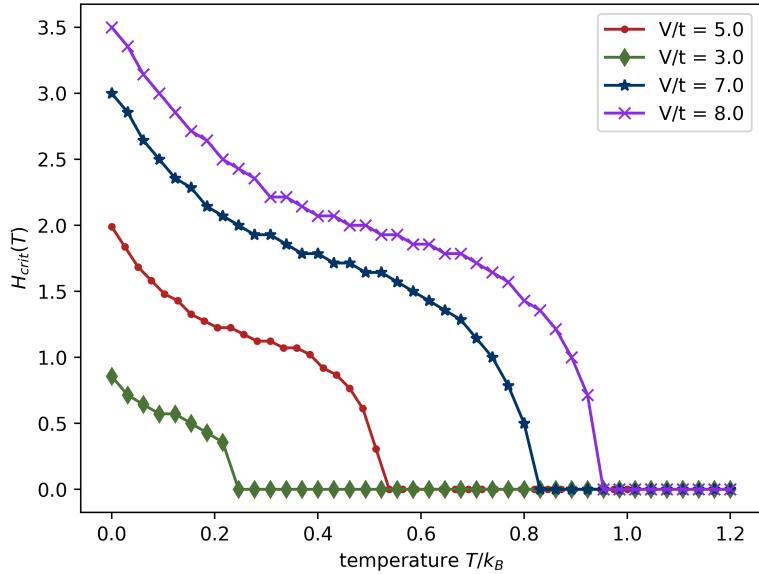
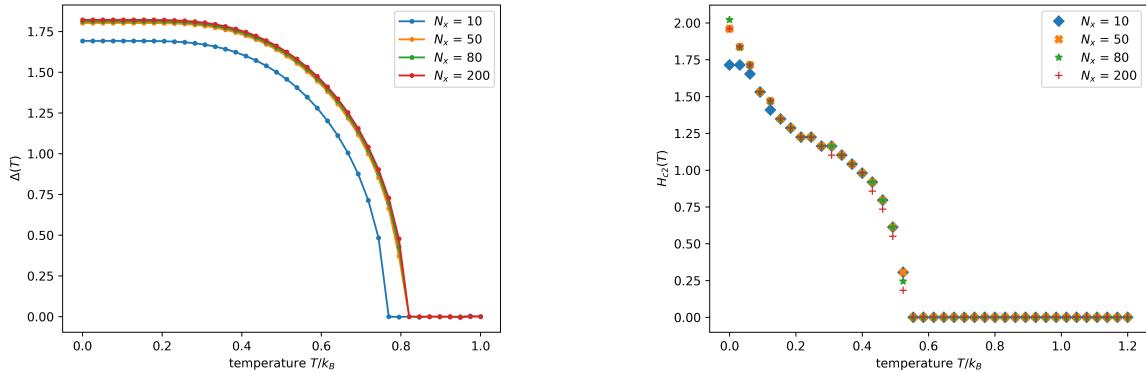


Figure 5: Calculation of the critical field H_{c2} for a 30×30 square lattice for different interaction strengths.

In Figure 6a we present the order parameter of the mean field problem as a function of temperature (not yet with magnetic coupling). We can already see from the simple problem that the order parameter $\Delta(T)$ converges to a specific curve with increasing system size. We use this result as an initial guess for the iterative solving when including the magnetic coupling. Let us check if we observe the same for the calculation on the BdG formalism. The result of that computation is plotted in Figure 6b.



(a) Plot of order parameter as a function of temperature for the mean field problem. We use $V/t = 5.0$.

(b) Calculation of H_{c2} for different system sizes and $V/t = 5.0$.

Figure 6: On the left we plot the order $\Delta(T)$ of the mean field for different system sizes. We use those results to compute the upper critical field $H_{c2}(T)$ (on the right). We see there is convergence of $H_{c2}(T)$ for increasing system size.

system size N_x	10	50	80	200
time	52 s	40 min	168 min	53 h

Table 1: Table of time periods needed for calculations of the upper critical field for different system sizes N_x .

This convergence is very convenient for us. In table 1 we listed the time periods for the computation of the critical field for different system sizes. As one can observe the duration increases drastically with system size but we obtain the same results for H_{c2} . This means we can stay at small system sizes and obtain the same physics for larger systems.

Previously, we have consistently plotted $H_{c2}(T)$ by incrementally increasing the magnetic field at a fixed temperature. We halted the algorithm upon the convergence of the order parameter to zero. We now perform a sanity check by computing $T_C(H)$, incrementally increasing the temperature while keeping the magnetic field constant. The results are plotted in Figure 7. We see that the curves coincide as expected.

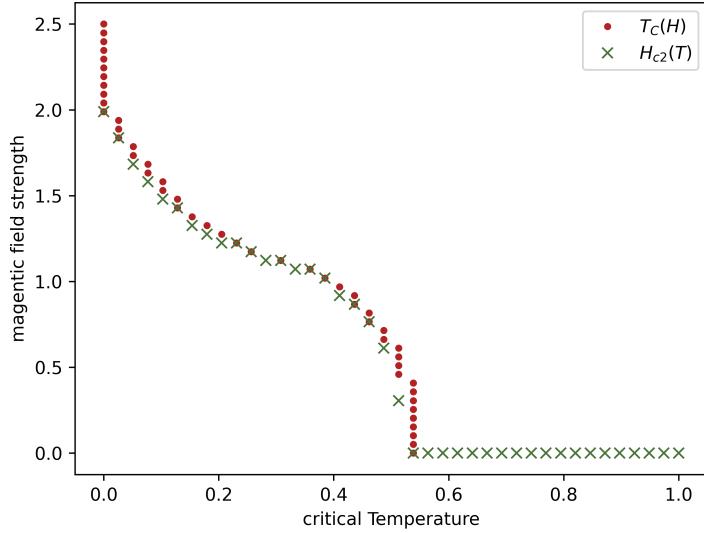
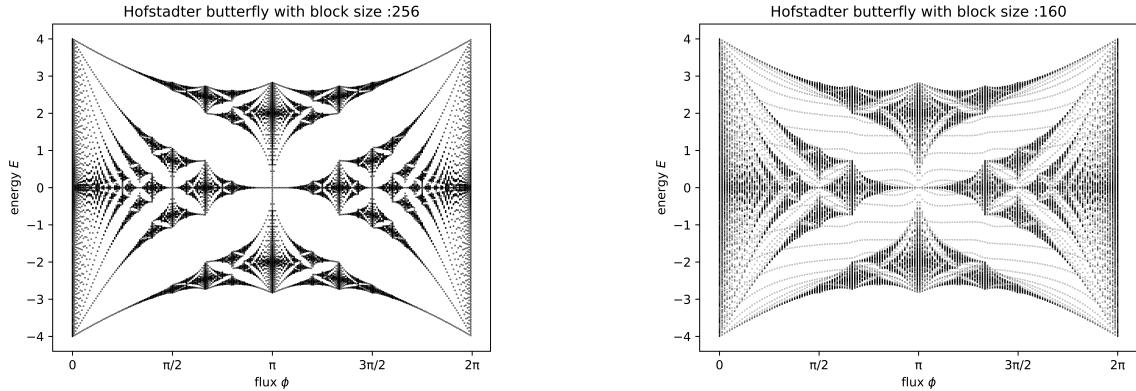


Figure 7: Plot of $T_C(H)$ and $H_{c2}(T)$. Quick explanation on how to read the graphs. The red one curve describes what is the critical temperature for a given magnetic field strength. The green one is the opposite, i.e., at what magnetic field strength vanishes the order parameter for a given temperature.

3.3.2 Critical H-field Analysis for Hofstadter Model

Let us discuss now the magnetic coupling via Peierls substitution, i.e., the Hofstadter model. We first plot the energy spectrum as a function of the magnetic flux ϕ where we once set periodic boundaries in x-direction (fig. 8a) and one time with open boundary conditions in x-direction (fig 8b). We obtain a spectrum of a self-similar structure called the Hofstadter butterfly. Next we can check if we can observe the Landau levels 2.2.1 for small magnetic fluxes. So we zoom in into the bottom left corner of Figure 8a. The zoomed in section is plotted in Figure 9. We can clearly see the evenly spaced points at low fluxes which confirms the Landau levels.



(a) Plot of energy spectrum of Hofstadter Hamiltonian (6) as a function of the magnetic flux with periodic boundary conditions.

(b) Plot of energy spectrum of Hofstadter Hamiltonian (6) as a function of the magnetic flux with open boundary conditions.

Figure 8: Self similar structure (called Hofstadter's butterfly) of the energy as a function of magnetic flux for the Hofstadter model (6) for different boundary conditions.

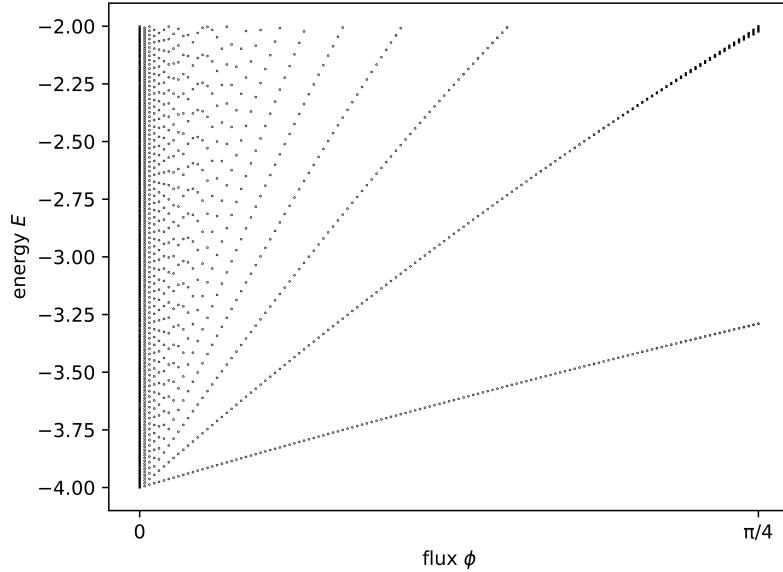


Figure 9: Zoomed in section of the Hofstadter butterfly with periodic boundary conditions of the bottom left corner of Figure 8a. We observe an even spacing of the energies at low magnetic fluxes which confirms the nature of the Landau levels.

This magnetic coupling through the electrons orbital motion has a drastic effect on the DOS of the system. The DOS gets significantly redistributed when we couple the electronic system to a magnetic field, as one can in Figures 10.

As we have described in section 2.2.1 the notable redistribution of the density of states corresponds exactly to the Landau levels.

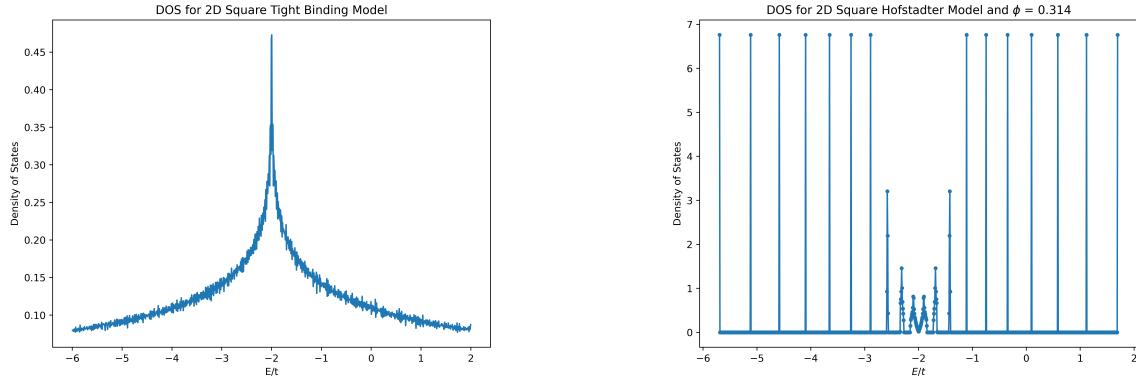


Figure 10: On the left we show the DOS of a tight binding model on a two dimensional lattice without magnetic field. On the right we include the magnetic response in form of the Peierls substitution with magnetic flux $\phi = 0.314$ through the unit cell.

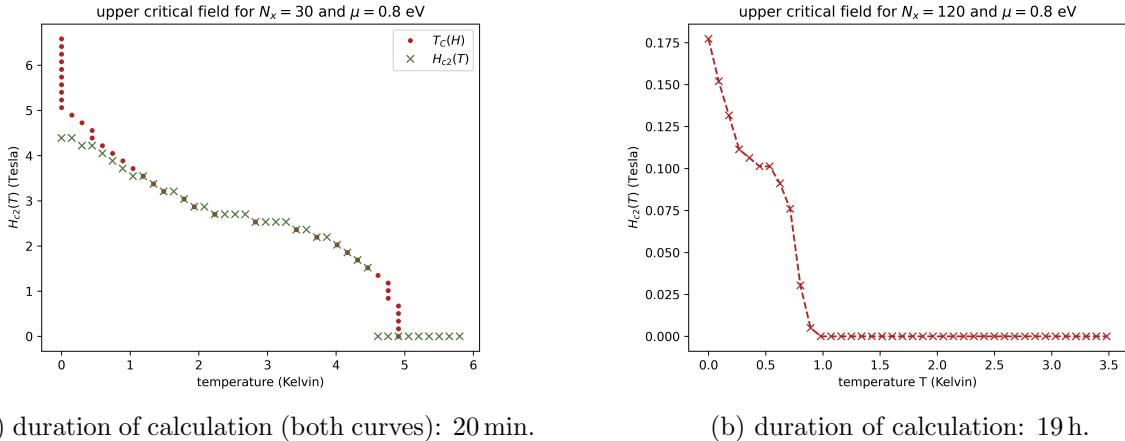
Up to this point, we have expressed the magnetic field and temperature in arbitrary units. Now, we aim to determine the upper critical field $H_{c2}(T)$ in SI units, where temperature will be measured in Kelvin and the magnetic field in Tesla.

The hopping constant t is determined by the overlap of atomic orbitals and the distance between them. For typical interatomic distances of approximately 1 \AA , t usually falls around 1 eV, which is also true for the potential strength V .

In the computation we consider the temperature $k_B T$ in units of energy (order of eV) and the magnetic field in dimensionless units. The conversion factors to SI units are the following,

$$1 \text{ eV} \rightarrow 11\,600 \text{ K}, \quad 1 \rightarrow 65\,821 \text{ T}.$$

In Figures 11a and 11b we present the results of the calculation of the upper critical field for $V/t = 0.5$ and $\mu = 0.8 \text{ eV}$ and system sizes $N_x = 30, 120$. We observe that the magnetic field strengths as well as the temperatures lay in reasonable range as one would expect from experiment. In Figure 11a we confirmed that the order of the two sweeps (magnetic field and temperature) is irrelevant, as the curves coincide.



(a) duration of calculation (both curves): 20 min.

(b) duration of calculation: 19 h.

Figure 11: Upper critical field computation for the Hofstadter model for the parameters $t = 1$ eV, $V = 0.5$ eV and $\mu = 0.8$ eV and for system sizes $N_x = 30, 120$.

Note that the $H_{c2}(T)$ changes significantly as a function of system sizes, indicating that, at least for $N_x = 30$, the results are not converged in system size.

For the left plot the red curve describes what is the critical temperature for a given magnetic field strength. The green one is the opposite, i.e., at what magnetic field strength vanishes the order parameter for a given temperature.

4 Conclusion

From the above discussion in section 3 we conclude that we successfully managed to compute the upper critical field of a two dimensional square lattice interacting with magnetic field via Zeeman coupling. From Figure 6 we make the assumption that considering smaller lattice sizes yields the same critical field as for larger sizes. This is a great advantage in terms of the duration of the calculation. Solving the self-consistency equation (30) is computationally intensive for large systems, as it requires repeatedly diagonalizing a $4N_x \times 4N_x$ matrix for each temperature and magnetic field configuration, where N_x is the number of lattice sites in one direction.

For numerical computations, we note that a custom iterative solver is preferable to the root-solving routines in *scipy*, as the latter are more time-consuming for one-dimensional cases and often fail to converge in two-dimensional cases.

Regarding the magnetic field response via Peierls substitution we have succeeded to determine the upper critical field too.

Additionally, we calculated the magnetic field strength and temperature in SI units, with results falling within a reasonable range, consistent with experimental expectations.

In summary, we established the basics for a numerical framework in order to determine the upper critical field.

This can be further extended by first combining both magnetic responses, and then incorporating a general pairing term. In other words, the order parameter matrix can adopt a more general form, without being restricted to a diagonal structure.

4.1 Comment on $T < T_C$ Computations

As it turns out we did not consider the full physical picture: below the critical temperature T_C , the magnetic field is screened inside the material due to the Meissner effect, which introduces additional complexity. Therefore our results for the critical magnetic field below the critical temperature do not capture the correct physics.

The applied method fails to reproduce the correct gap function for $T < T_C$ because it neglects the induced currents and the resulting magnetic field screening. However, when evaluating $H_{c2}(T)$, we are primarily interested at the configuration of temperature and field strength where we first encounter a non-trivial gap function.

In that sense, our method should still reproduce the correct results for H_{c2} .

One could check the values obtained for the critical temperature with the solutions of the linearized gap equation. Unfortunately, we were not able to do this because the algorithm for the linearized gap equation was unstable and did not return any eigenvalues with the value 1.

For further investigations one should use a linearized gap equation in order to determine the critical temperature T_C , as it is described in section 2.6, since it requires diagonalizing a matrix only once for each magnetic field configuration.

5 Acknowledgement

I acknowledge Dr. Mark Fischer and Bernhard Lüscher for providing me the opportunity to conduct this semester project. Special thanks to Bernhard Lüscher for supervising the project as well as the many profound discussions and helpful tips and tricks.

6 References

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A Derivations

In this subsection, we provide the derivations on how to transform certain Hamiltonian partially into Fourier space. In other words our considered Hamiltonians have simultaneously open boundaries in one dimension as well as periodic boundaries in another direction. We restrict our analysis on a square (2D) lattice and set the lattice constants $a_x = a_y = 1$ for simplicity.

A.1 tight binding Hamiltonian

The general form of a Hamiltonian of a tight binding is given by

$$H = \sum_{\langle i,j \rangle, \sigma} -t_{ij} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{h.c.} - \mu \sum_{i,\sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma}. \quad (33)$$

For simplicity we assume the model to be spinless and we set $\mu = 0$.

In the following we assume the tunneling constant to be constant, i.e., $t_{ij} = t$. Now we want to transform the Hamiltonian into Fourier space but only in y -direction. In order to do that we use the following identities

$$\hat{c}_{x_i, y_j} = \frac{1}{\sqrt{N_y}} \sum_{k_y} e^{-ik_y y_j} \hat{c}_{x_i, k_y}, \quad \text{and} \quad \frac{1}{N_y} \sum_{r_{i_y}} e^{-ir_{i_y} (k_y - k'_y)} = \delta_{k_y, k'_y}. \quad (34)$$

Performing the Fourier transform we obtain

$$\begin{aligned} H &= -t \cdot \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j \\ &= -\frac{t}{2} \sum_{i_x, i_y} \left(\hat{c}_{i_x, i_y}^\dagger \hat{c}_{i_x+1, i_y} + \hat{c}_{i_x, i_y}^\dagger \hat{c}_{i_x, i_y+1} + \hat{c}_{i_x, i_y}^\dagger \hat{c}_{i_x-1, i_y} + \hat{c}_{i_x, i_y}^\dagger \hat{c}_{i_x, i_y-1} + \text{h.c.} \right) \end{aligned} \quad (35)$$

$$\stackrel{\text{FT}}{=} \frac{-t}{2} \sum_{i_x, k_y} \left(\hat{c}_{i_x, k_y}^\dagger \hat{c}_{i_x+1, k_y} + \hat{c}_{i_x, k_y}^\dagger \hat{c}_{i_x-1, k_y} + \text{h.c.} \right) + 2 \cdot \left(e^{ik_y} + e^{-ik_y} \right) \hat{c}_{i_x, k_y}^\dagger \hat{c}_{i_x, k_y}. \quad (36)$$

Now written out in matrix form

$$H = -t \cdot \sum_{k_y} \left(\hat{c}_{1, k_y}^\dagger, \hat{c}_{2, k_y}^\dagger, \hat{c}_{3, k_y}^\dagger, \dots \right) \begin{pmatrix} 2 \cos(k_y) & 1 & & & 1/0 \\ 1 & 2 \cos(k_y) & 1 & & \\ & 1 & 2 \cos(k_y) & 1 & \\ & & 1 & \ddots & \ddots \\ 1/0 & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \hat{c}_{1, k_y} \\ \hat{c}_{2, k_y} \\ \hat{c}_{3, k_y} \\ \vdots \end{pmatrix}. \quad (37)$$

We observe that in the edge entries of the antidiagonal can take on two distinct values depending on the boundary conditions of our system. They are 1 for periodic boundaries or 0 for open boundary conditions.

A.2 tight binding with Zeeman coupling

The Hamiltonian we consider here is a tight binding Hamiltonian, like in equation (33), with an additional coupling term which looks like

$$\hat{H}_Z = -\frac{B}{2} \sum_{i,\sigma,\sigma'} \hat{c}_{i,\sigma}^\dagger \hat{\sigma}_{\sigma,\sigma'}^z \hat{c}_{i,\sigma'}. \quad (38)$$

Here we implicitly assumed that the magnetic field is constant and aligned along the z-axis, i.e., $\vec{B} = (0, 0, B)$.

We again do the Fourier transform in y-direction

$$\hat{H}_Z = -\frac{B}{2} \sum_{i_x, k_y, \sigma, \sigma'} \hat{\sigma}_{\sigma, \sigma'}^z \hat{c}_{i_x, k_y, \sigma}^\dagger \hat{c}_{i_x, k_y, \sigma'} = -\frac{B}{2} \sum_{i_x, k_y} \hat{c}_{i_x, k_y, \uparrow}^\dagger \hat{c}_{i_x, k_y, \uparrow} - \hat{c}_{i_x, k_y, \downarrow}^\dagger \hat{c}_{i_x, k_y, \downarrow} \quad (39)$$

where in the last equality we used that $\hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

A.3 Hofstadter Hamiltonian

The Hofstadter Hamiltonian in real space is given by:

$$\hat{H}_{Hof} = - \sum_{\langle i, j \rangle} \left(\tilde{t}_{ij} \hat{c}_{x_i, y_j}^\dagger \hat{c}_{x_i, y_j} + \text{h.c.} \right). \quad (40)$$

Now our Hamiltonian is periodic in y-direction and has open boundaries in x direction, so we Fourier transform it but only in y-direction. For the annihilation operator it holds

$$\hat{c}_{x_i, y_j} = \frac{1}{\sqrt{N_y}} \sum_{k_y} e^{-ik_y y_j} \hat{c}_{x_i, k_y}. \quad (41)$$

Additionally the \tilde{t}_{ij} has the form $\tilde{t}_{ij} = t \cdot e^{-i \int_{r_i}^{r_j} \vec{A} \cdot d\vec{r}}$. Thus our Hamiltonian becomes

$$\begin{aligned} \hat{H}_{Hof} &= -t \cdot \sum_{i, j} \left(\hat{c}_{x_i+1, y_j}^\dagger \hat{c}_{x_i, y_j} + \text{h.c.} \right) + e^{-iBx_i} \hat{c}_{x_i, y_j+1}^\dagger \hat{c}_{x_i, y_j} + e^{iBx_i} \hat{c}_{x_i, y_j}^\dagger \hat{c}_{x_i, y_j+1} \\ &= -t \cdot \sum_{i, k} \left(\hat{c}_{x_i+1, k}^\dagger \hat{c}_{x_i, k} + \text{h.c.} \right) + e^{-i(Bx_i - k)} \hat{c}_{x_i, k}^\dagger \hat{c}_{x_i, k} + e^{i(Bx_i - k)} \hat{c}_{x_i, k}^\dagger \hat{c}_{x_i, k} \\ &= -t \cdot \sum_{i, k} \left(\hat{c}_{x_i+1, k}^\dagger \hat{c}_{x_i, k} + \text{h.c.} \right) + 2 \cos(k - Bx_i) \hat{c}_{x_i, k}^\dagger \hat{c}_{x_i, k}. \end{aligned}$$