Title of the Thesis

Author's name

Masterarbeit in Physik
angefertigt im Helmholtz-Institut für Strahlen- und Kernphysik

vorgelegt der
Mathematisch-Naturwissenschaftlichen Fakultät
der
Rheinischen Friedrich-Wilhelms-Universität
Bonn

MMM 2021

I hereby declare that this thesis was formulated by myself and that no sources or tools other than those cited were used.

Bonn, ...
Date Signature

1. Gutachter: Prof. Dr. John Smith
2. Gutachterin: Prof. Dr. Anne Jones

Acknowledgements

I would like to thank ...

You should probably use `\chapter*` for acknowledgements at the beginning of a thesis and `\chapter` for the end.

Contents

CHAPTER 1

Introduction

The introduction usually gives a few pages of introduction to the whole subject, maybe even starting with the Greeks.

For more information on LaTeX and the packages that are available see for example the books of Kopka [1] and Goossens et al [2].

A lot of useful information on particle physics can be found in the "Particle Data Book" [3].

I have resisted the temptation to put a lot of definitions into the file `thesis_defs.sty`, as everyone has their own taste as to what scheme they want to use for names. However, a few examples are included to help you get started:

- cross-sections are measured in pb and integrated luminosity in pb^{-1};
- the K_S^0 is an interesting particle;
- the missing transverse momentum, $p_{\mathrm{T}}^{\mathrm{miss}}$, is often called missing transverse energy, even though it is calculated using a vector sum.

Note that the examples of units assume that you are using the siunitx package.

It also is probably a good idea to include a few well formatted references in the thesis skeleton. More detailed suggestions on what citation types to use can be found in the "Thesis Guide" [4]:

- articles in refereed journals [3, 5];
- a book [6];
- a PhD thesis [7] and a Diplom thesis [8];
- a collection of articles [9];
- a conference note [10];
- a preprint [11] (you can also use `@online` or `@booklet` for such things);
- something that is only available online [4].

At the end of the introduction it is normal to say briefly what comes in the following chapters.

The line at the beginning of this file is used by TeXstudio etc. to specify which is the master LaTeX file, so that you can compile your thesis directly from this file. If your thesis is called something other than `mythesis`, adjust it as appropriate.

CHAPTER 2

Theoretical Overview

2.1 Excitons

2.2 The Hubbard Model

The Hubbard model (HM) emerges as a simple solution to the many-body problem in solids. It is a theory that describes the interactions of fermions on lattices, where they can hop between neighboring sites. This model successfully describes the feromagnetic properties of materials with different strength correlations between electrons.

The tight-binding with on-site interaction hamiltonian desribes the hopping of the fermions between neighboring sites and the interaction of fermions

$$H = -\sum_{xy}\left(a^{\dagger}_{x,\uparrow}K_{xy}a_{y,\uparrow} + a^{\dagger}_{x,\downarrow}K_{xy}a_{y,\downarrow}\right) - \frac{1}{2}\sum_{x,y}\left((n^{\dagger}_{x,\uparrow} - n^{\dagger}_{x,\downarrow})V_{xy}(n^{\dagger}_{y,\uparrow} - n^{\dagger}_{y,\downarrow})\right) \tag{2.1}$$

where the first term is the kinetic and the second is the interaction; $a^{\dagger}$, a are the creation and annihilation operators respectively of electrons, $\uparrow$ is indicating spin-up and $\downarrow$ is spin-down, K is called the hopping matrix which describes the hopping between sites, the interaction term is represented by the potential V, and $n_{x,s} = a^{\dagger}_{x,s}a_{x,s}$ is the electron number density operator. We can make a change of basis, such that particles are separated by spin and charge, which we call a particle-hole symmetry (see Section **??**)

$$\begin{aligned} p^{\dagger}_{x} &\equiv a^{\dagger}_{x,\uparrow} \qquad & h^{\dagger}_{x} &\equiv a_{x,\downarrow} \\ p_{x} &\equiv a_{x,\uparrow} \qquad & h_{x} &\equiv a^{\dagger}_{x,\downarrow} \end{aligned} \tag{2.2}$$

where $p^{\dagger}(p)$, $h^{\dagger}(h)$ are the creation(annihilation) operators of particles and holes. Since these operators describe fermions, they respect the anti-commutation relations i.e. the Pauli exclusion principle

$$\begin{aligned} \{p^{\dagger}_{x}, p_{y}\} &= \delta_{xy} & \{h^{\dagger}_{x}, h_{y}\} &= \delta_{xy} \\ \{p_{x}, p_{y}\} &= \{p^{\dagger}_{x}, p^{\dagger}_{y}\} = 0 & \{h_{x}, h_{y}\} &= \{h^{\dagger}_{x}, h^{\dagger}_{y}\} = 0 \\ \{p^{\dagger}_{x}, p_{y}\} &= \{p^{\dagger}_{x}, h^{\dagger}_{y}\} = 0 & \{p_{x}, h_{y}\} &= \{p_{x}, h^{\dagger}_{y}\} = 0 \end{aligned} \tag{2.3}$$

The convention for spin and charge that we use for the particles and holes operators is given in Table 2.1. Here Q, S, S^3 are the charge, spin, and the third component of the spin respectively. For the

	Q	S	S^3
$p^\dagger$	+1	$\frac{1}{2}$	$-\frac{1}{2}$
p	-1	$\frac{1}{2}$	$+\frac{1}{2}$
$h^\dagger$	-1	$\frac{1}{2}$	$-\frac{1}{2}$
h	+1	$\frac{1}{2}$	$+\frac{1}{2}$

Table 2.1: Convention of charge (Q), spin (S), and third component of spin (S^3) used for creation and annihilation operators of particles and holes.

two-body correlators (discussed in Section 2.4), it is also convinient to know the quantum numbers for different combinations of particle and hole operators. In Table 2.2 is given a summary which will be useful in the next chapters. We notice that only the charge and S^3 are present in the table. This is due to Q and S^3 being additive numbers, whereas the spin is not because two different spin values could have the same third component (ex. $S = 0, 1; S^3 = 0$).

	Q	S^3
$p^\dagger p^\dagger$	+2	-1
$p^\dagger p$	0	0
$p^\dagger h^\dagger$	0	-1
$p^\dagger h$	+2	0
pp	-2	+1
$ph^\dagger$	-2	0
ph	0	+1
$h^\dagger h^\dagger$	-2	-1
$h^\dagger h$	0	0
hh	+2	+1

Table 2.2: Quantum numbers for the combination of particle and hole operators.

We can now substitute the operators inside the hamiltonian with the ones in the new basis

$$H = -\sum_{xy} \left(p_x^\dagger K_{xy} p_y - h_x^\dagger K_{xy} h_y \right) + \frac{1}{2} \sum_{x,y} \left((n_{x,p}^\dagger - n_{x,h}^\dagger) V_{xy} (n_{y,p}^\dagger - n_{y,h}^\dagger) \right), \tag{2.4}$$

here we have added a new index to the number density operators which indicates whether particles or holes are counted.

Finally, we can expand our hamiltonian with one more term which is called the chemical potential term, where μ is the chemical potential. It accounts for the change of the number of particles and holes

$$H - \vec{\mu} \cdot \vec{q} = -\sum_{xy} \left(p_x^\dagger K_{xy} p_y + h_x^\dagger K_{xy} h_y \right) + \frac{1}{2} \sum_{xy} q_x V_{xy} q_y - \sum_x \mu_x q_x \tag{2.5}$$

and we have introduced one more operator $q_x = n_{x,p} - n_{x,h}$. This is the charge operator that indicates the relative charge on each site.

The hamiltonian of this model for our ease can be devided into two parts – the half-filling part of the whole hamiltonian and the chemical potential part. The former contains the kinetic and the interaction terms whereas the latter in made out of only the chemical term. In the case of bipartite lattices (Chapter "SYMMETRY"), we must be able to differentiate on which lattice sites the operators are. This could be done by modifying the transformation (2.2) to include site dependent sign σ_k for holes

$$H - \vec{\mu} \cdot \vec{q} = -\sum_{xy} \left(p_x^\dagger K_{xy} p_y + \sigma_k h_x^\dagger K_{xy} h_y \right) + \frac{1}{2} \sum_{xy} q_x V_{xy} q_y - \sum_x \mu_x q_x. \tag{2.6}$$

To get to the hamiltonian that we work with, we choose to have only contact interactions ($V_{xy} = U\delta_{xy}$). This means that the interactions are done only in the same site

$$H - \vec{\mu} \cdot \vec{q} = -\sum_{xy} \left(p_x^\dagger K_{xy} p_y + \sigma_k h_x^\dagger K_{xy} h_y \right) + \frac{U}{2} \sum_{xy} q_x^2 - \sum_x \mu_x q_x. \tag{2.7}$$

In this thesis work we sometimes work with the chemical potential and sometimes we set $\mu = 0$, depending on the symmetries that we use [**avoiding ergodicity**]. On Figure 2.1 is shown a schematic of the Hubbard model's hopping and interaction. The theory that we are working with as mentioned

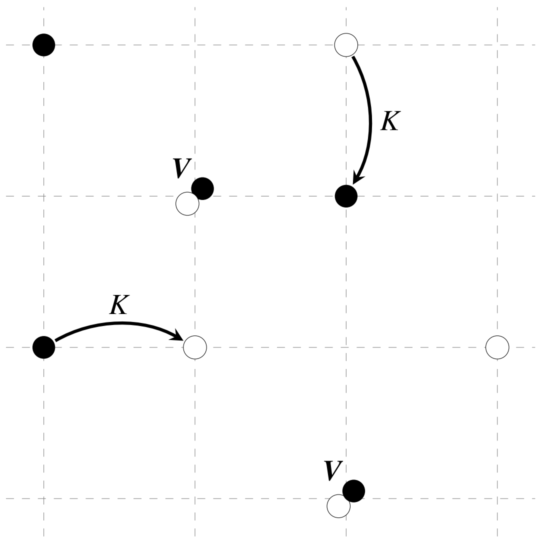

Figure 2.1: Schematic view of the hopping and the interaction of electrons with different spin on a square lattice. Here K is the hopping matrix containing the hopping probabilities and V is the interaction potential. In the particle-hole basis the black and white dots represent particles and holes.

before is a model of the real physical systems. Even though the HM gives us good results, one must know some of the drawbacks of the model. One is that it neglects the long range part of the Coulomb forces. It is likely that significant effects are missed by this simplification [MOTT]. Another weakness of this model it has difficulties being applied to transition metals. And the Hubbard model cannot be exactly solved, so approximations must be used.

Despite having these issues, the two-dimensional HM has showed promising results when applied to honeycomb lattices. The description of the electronic structure when applied resemble that of the carbon nano structures, such as graphene, carbon nano tubes, and ribbons.

2.3 HMC

2.4 Corelation Functions

CHAPTER 3

Symmetries

3.1 Correlation functions

3.1.1 One-particle correlation function

We start with correlator $\langle phh^\dagger p^\dagger \rangle$

$$C_{Q=0,S=1,S^3=+1;k,q,r,s} = \begin{bmatrix} p_+h_+h_+^\dagger p_+^\dagger & p_+h_+h_+^\dagger p_-^\dagger & p_+h_+h_-^\dagger p_+^\dagger & p_+h_+h_-^\dagger p_-^\dagger \\ p_+h_-h_+^\dagger p_+^\dagger & p_+h_-h_+^\dagger p_-^\dagger & p_+h_-h_-^\dagger p_+^\dagger & p_+h_-h_-^\dagger p_-^\dagger \\ p_-h_+h_+^\dagger p_+^\dagger & p_-h_+h_+^\dagger p_-^\dagger & p_-h_+h_-^\dagger p_+^\dagger & p_-h_+h_-^\dagger p_-^\dagger \\ p_-h_-h_+^\dagger p_+^\dagger & p_-h_-h_+^\dagger p_-^\dagger & p_-h_-h_-^\dagger p_+^\dagger & p_-h_-h_-^\dagger p_-^\dagger \end{bmatrix}_{k,q,r,s} (\tau)$$

Now, we apply different symmetry operator to the two particle correlation funtion. When we apply them, we first start with the thermal trace and then switch to matrix form, so that it is easier to see the transformations needed in order to get another two particle correlator.

We obviously start with the trace cyclicity.

$$C_{Q=0,S=1,S^3=+1;k,q,r,s} = \frac{1}{Z} tr \left[p_k h_q e^{-H\tau} h_r^\dagger p_s^\dagger e^{-H(\beta-\tau)} \right] = \frac{1}{Z} tr \left[h_r^\dagger p_s^\dagger e^{-H(\beta-\tau)} p_k h_q e^{-H\tau} \right]$$

Now we apply time reverse

$$\beta \to \beta - \tau$$

and use the anti-commutation relations of the operators to get

$$\frac{1}{Z} tr \left[h_r^\dagger p_s^\dagger e^{-H(\beta-(\beta-\tau))} p_k h_q e^{-H(\beta-\tau)} \right] = \frac{1}{Z} tr \left[p_s^\dagger h_r^\dagger e^{-H\tau} h_q p_k e^{-H(\beta-\tau)} \right] \tag{3.1}$$

Now we switch to matrix form to see better what happens.

$$C_{Q=0,S=1,S^3=+1;k,q,r,s}$$

$$= \begin{bmatrix} p_+h_+h_+^\dagger p_+^\dagger & p_+h_+h_+^\dagger p_-^\dagger & p_+h_+h_-^\dagger p_+^\dagger & p_+h_+h_-^\dagger p_-^\dagger \\ p_+h_-h_+^\dagger p_+^\dagger & p_+h_-h_+^\dagger p_-^\dagger & p_+h_-h_-^\dagger p_+^\dagger & p_+h_-h_-^\dagger p_-^\dagger \\ p_-h_+h_+^\dagger p_+^\dagger & p_-h_+h_+^\dagger p_-^\dagger & p_-h_+h_-^\dagger p_+^\dagger & p_-h_+h_-^\dagger p_-^\dagger \\ p_-h_-h_+^\dagger p_+^\dagger & p_-h_-h_+^\dagger p_-^\dagger & p_-h_-h_-^\dagger p_+^\dagger & p_-h_-h_-^\dagger p_-^\dagger \end{bmatrix}_{k,q,r,s} (\tau)$$

$$= \begin{bmatrix} h_+^\dagger p_+^\dagger p_+h_+ & h_+^\dagger p_-^\dagger p_+h_+ & h_-^\dagger p_+^\dagger p_+h_+ & h_-^\dagger p_-^\dagger p_+h_+ \\ h_+^\dagger p_+^\dagger p_+h_- & h_+^\dagger p_-^\dagger p_+h_- & h_-^\dagger p_+^\dagger p_+h_- & h_-^\dagger p_-^\dagger p_+h_- \\ h_+^\dagger p_+^\dagger p_-h_+ & h_+^\dagger p_-^\dagger p_-h_+ & h_-^\dagger p_+^\dagger p_-h_+ & h_-^\dagger p_-^\dagger p_-h_+ \\ h_+^\dagger p_+^\dagger p_-h_- & h_+^\dagger p_-^\dagger p_-h_- & h_-^\dagger p_+^\dagger p_-h_- & h_-^\dagger p_-^\dagger p_-h_- \end{bmatrix}_{r,s,k,q} (\beta-\tau)$$

$$= \begin{bmatrix} p_+^\dagger h_+^\dagger h_+p_+ & p_-^\dagger h_+^\dagger h_+p_+ & p_+^\dagger h_-^\dagger h_+p_+ & p_-^\dagger h_-^\dagger h_+p_+ \\ p_+^\dagger h_+^\dagger h_-p_+ & p_-^\dagger h_+^\dagger h_-p_+ & p_+^\dagger h_-^\dagger h_-p_+ & p_-^\dagger h_-^\dagger h_-p_+ \\ p_+^\dagger h_+^\dagger h_+p_- & p_-^\dagger h_+^\dagger h_+p_- & p_+^\dagger h_-^\dagger h_+p_- & p_-^\dagger h_-^\dagger h_+p_- \\ p_+^\dagger h_+^\dagger h_-p_- & p_-^\dagger h_+^\dagger h_-p_- & p_+^\dagger h_-^\dagger h_-p_- & p_-^\dagger h_-^\dagger h_-p_- \end{bmatrix}_{s,r,q,k} (\beta-\tau) = C_{Q=0,S=1,S^3=-1;s,r,q,k}$$

We can notice that order reverse is actually a composed of two transformations – particle-hole momentum switch and time reverse. After we stare at the matrix for an hour, we can figure out what the transformation between the correlation functions is.

$$C_{Q=0,S=1,S^3=+1;k,q,r,s}(\tau) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} C_{Q=0,S=1,S^3=-1;s,r,q,k}{}^\top(\beta-\tau) \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

We repeat the steps again for each symmetry operator. First we start with the thermal trace and then switch to matrix for easy transformations.

$I : H - \vec{\mu} \cdot \vec{q}$

$$\begin{aligned} &C_{Q=0,S=1,S^3=+1;k,q,r,s} \\ &= \frac{1}{Z} tr\left[p_k h_q e^{-H\tau} h_r^\dagger p_s^\dagger e^{-H(\beta-\tau)}\right] \\ &= \frac{1}{Z} tr\left[I^{-1} I p_k I^{-1} I h_q I^{-1} I e^{-H\tau} I^{-1} I h_r^\dagger I^{-1} I p_s^\dagger I^{-1} I e^{-H(\beta-\tau)}\right] \\ &= \frac{1}{Z} tr\left[I p_k I^{-1} I h_q I^{-1} I e^{-H\tau} I^{-1} I h_r^\dagger I^{-1} I p_s^\dagger I^{-1} I e^{-H(\beta-\tau) I^{-1}}\right] \\ &= \frac{1}{Z} tr\left[(\Sigma h)_k^\dagger (\Sigma p)_q^\dagger e^{-H\tau} (\Sigma p)_r (\Sigma h)_s e^{-H(\beta-\tau)}\right] \\ &= \frac{1}{Z} tr\left[(\Sigma p)_q^\dagger (\Sigma h)_k^\dagger e^{-H\tau} (\Sigma h)_s (\Sigma p)_r e^{-H(\beta-\tau)}\right] \end{aligned}$$

$$
\begin{aligned}
&C_{Q=0,S=1,S^3=+1;k,q,r,s} \\
&= I^{-1} \begin{bmatrix} p_+h_+h_+^\dagger p_+^\dagger & p_+h_+h_+^\dagger p_-^\dagger & p_+h_+h_-^\dagger p_+^\dagger & p_+h_+h_-^\dagger p_-^\dagger \\ p_+h_-h_+^\dagger p_+^\dagger & p_+h_-h_+^\dagger p_-^\dagger & p_+h_-h_-^\dagger p_+^\dagger & p_+h_-h_-^\dagger p_-^\dagger \\ p_-h_+h_+^\dagger p_+^\dagger & p_-h_+h_+^\dagger p_-^\dagger & p_-h_+h_-^\dagger p_+^\dagger & p_-h_+h_-^\dagger p_-^\dagger \\ p_-h_-h_+^\dagger p_+^\dagger & p_-h_-h_+^\dagger p_-^\dagger & p_-h_-h_-^\dagger p_+^\dagger & p_-h_-h_-^\dagger p_-^\dagger \end{bmatrix}_{k,q,r,s} (\tau)\ I \\
&= \begin{bmatrix} (\Sigma h)_+^\dagger (\Sigma p)_+^\dagger (\Sigma p)_+ (\Sigma h)_+ & (\Sigma h)_+^\dagger (\Sigma p)_+^\dagger (\Sigma p)_+ (\Sigma h)_- & (\Sigma h)_+^\dagger (\Sigma p)_+^\dagger (\Sigma p)_- (\Sigma h)_+ & (\Sigma h)_+^\dagger (\Sigma p)_+^\dagger (\Sigma p)_- (\Sigma h)_- \\ (\Sigma h)_+^\dagger (\Sigma p)_-^\dagger (\Sigma p)_+ (\Sigma h)_+ & (\Sigma h)_+^\dagger (\Sigma p)_-^\dagger (\Sigma p)_+ (\Sigma h)_- & (\Sigma h)_+^\dagger (\Sigma p)_-^\dagger (\Sigma p)_- (\Sigma h)_+ & (\Sigma h)_+^\dagger (\Sigma p)_-^\dagger (\Sigma p)_- (\Sigma h)_- \\ (\Sigma h)_-^\dagger (\Sigma p)_+^\dagger (\Sigma p)_+ (\Sigma h)_+ & (\Sigma h)_-^\dagger (\Sigma p)_+^\dagger (\Sigma p)_+ (\Sigma h)_- & (\Sigma h)_-^\dagger (\Sigma p)_+^\dagger (\Sigma p)_- (\Sigma h)_+ & (\Sigma h)_-^\dagger (\Sigma p)_+^\dagger (\Sigma p)_- (\Sigma h)_- \\ (\Sigma h)_-^\dagger (\Sigma p)_-^\dagger (\Sigma p)_+ (\Sigma h)_+ & (\Sigma h)_-^\dagger (\Sigma p)_-^\dagger (\Sigma p)_+ (\Sigma h)_- & (\Sigma h)_-^\dagger (\Sigma p)_-^\dagger (\Sigma p)_- (\Sigma h)_+ & (\Sigma h)_-^\dagger (\Sigma p)_-^\dagger (\Sigma p)_- (\Sigma h)_- \end{bmatrix} \\
&= \begin{bmatrix} h_-^\dagger p_-^\dagger p_-h_- & h_-^\dagger p_-^\dagger p_-h_+ & h_-^\dagger p_-^\dagger p_+h_- & h_-^\dagger p_-^\dagger p_+h_+ \\ h_-^\dagger p_+^\dagger p_-h_- & h_-^\dagger p_+^\dagger p_-h_+ & h_-^\dagger p_+^\dagger p_+h_- & h_-^\dagger p_+^\dagger p_+h_+ \\ h_+^\dagger p_-^\dagger p_-h_- & h_+^\dagger p_-^\dagger p_-h_+ & h_+^\dagger p_-^\dagger p_+h_- & h_+^\dagger p_-^\dagger p_+h_+ \\ h_+^\dagger p_+^\dagger p_-h_- & h_+^\dagger p_+^\dagger p_-h_+ & h_+^\dagger p_+^\dagger p_+h_- & h_+^\dagger p_+^\dagger p_+h_+ \end{bmatrix}_{k,q,r,s} (\tau)
\end{aligned}
$$

$$
= \begin{bmatrix} p_-h_-h_-^\dagger p_-^\dagger & p_-h_+h_-^\dagger p_-^\dagger & p_+h_-h_-^\dagger p_-^\dagger & p_+h_+h_-^\dagger p_-^\dagger \\ p_-h_-h_-^\dagger p_+^\dagger & p_-h_+h_-^\dagger p_+^\dagger & p_+h_-h_-^\dagger p_+^\dagger & p_+h_+h_-^\dagger p_+^\dagger \\ p_-h_-h_+^\dagger p_-^\dagger & p_-h_+h_+^\dagger p_-^\dagger & p_+h_-h_+^\dagger p_-^\dagger & p_+h_+h_+^\dagger p_-^\dagger \\ p_-h_-h_+^\dagger p_+^\dagger & p_-h_+h_+^\dagger p_+^\dagger & p_+h_-h_+^\dagger p_+^\dagger & p_+h_+h_+^\dagger p_+^\dagger \end{bmatrix}_{r,s,k,q} (\beta-\tau)
$$

$$
= \begin{bmatrix} p_-^\dagger h_-^\dagger h_-p_- & p_-^\dagger h_-^\dagger h_+p_- & p_-^\dagger h_-^\dagger h_-p_+ & p_-^\dagger h_-^\dagger h_+p_+ \\ p_+^\dagger h_-^\dagger h_-p_- & p_+^\dagger h_-^\dagger h_+p_- & p_+^\dagger h_-^\dagger h_-p_+ & p_+^\dagger h_-^\dagger h_+p_+ \\ p_-^\dagger h_+^\dagger h_-p_- & p_-^\dagger h_+^\dagger h_+p_- & p_-^\dagger h_+^\dagger h_-p_+ & p_-^\dagger h_+^\dagger h_+p_+ \\ p_+^\dagger h_+^\dagger h_-p_- & p_+^\dagger h_+^\dagger h_+p_- & p_+^\dagger h_+^\dagger h_-p_+ & p_+^\dagger h_+^\dagger h_+p_+ \end{bmatrix}_{q,k,s,r} (\tau)
$$

Depending on what transformation we use to get back to $\langle phh^\dagger p^\dagger \rangle$, we get two transformations which are time reverse to one another. We notice the same behaviour for all operators.

$$
\begin{aligned}
&C_{Q=0,S=1,S^3=+1;k,q,r,s}(\tau) \\
&\qquad = \begin{bmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{bmatrix} C_{Q=0,S=1,S^3=+1;r,s,k,q}{}^\top(\beta-\tau) \begin{bmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
&C_{Q=0,S=1,S^3=+1;k,q,r,s}(\tau) \\
&\qquad = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{bmatrix} C_{Q=0,S=1,S^3=-1;q,k,s,r}(\tau) \begin{bmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}
\end{aligned}
$$

$C : H$

$$
\begin{aligned}
&C_{Q=0,S=1,S^3=+1;k,q,r,s}\\
&=\frac{1}{Z}tr\left[p_k h_q e^{-H\tau} h_r^\dagger p_s^\dagger e^{-H(\beta-\tau)}\right]\\
&=\frac{1}{Z}tr\left[C^{-1}Cp_kC^{-1}Ch_qC^{-1}Ce^{-H\tau}C^{-1}Ch_r^\dagger C^{-1}Cp_s^\dagger C^{-1}Ce^{-H(\beta-\tau)}\right]\\
&=\frac{1}{Z}tr\left[h_k p_q e^{-H\tau} p_r^\dagger h_s^\dagger e^{-H(\beta-\tau)}\right]\\
&=\frac{1}{Z}tr\left[p_q h_k e^{-H\tau} h_s^\dagger p_r^\dagger e^{-H(\beta-\tau)}\right]
\end{aligned}
$$

$$
\begin{aligned}
&C_{Q=0,S=1,S^3=+1;k,q,r,s}\\
&=C^{-1}\begin{bmatrix}
p_+h_+h_+^\dagger p_+^\dagger & p_+h_+h_+^\dagger p_-^\dagger & p_+h_+h_-^\dagger p_+^\dagger & p_+h_+h_-^\dagger p_-^\dagger\\
p_+h_-h_+^\dagger p_+^\dagger & p_+h_-h_+^\dagger p_-^\dagger & p_+h_-h_-^\dagger p_+^\dagger & p_+h_-h_-^\dagger p_-^\dagger\\
p_-h_+h_+^\dagger p_+^\dagger & p_-h_+h_+^\dagger p_-^\dagger & p_-h_+h_-^\dagger p_+^\dagger & p_-h_+h_-^\dagger p_-^\dagger\\
p_-h_-h_+^\dagger p_+^\dagger & p_-h_-h_+^\dagger p_-^\dagger & p_-h_-h_-^\dagger p_+^\dagger & p_-h_-h_-^\dagger p_-^\dagger
\end{bmatrix}_{k,q,r,s}(\tau)\,C
\end{aligned}
$$

$$
=\begin{bmatrix}
h_+p_+p_+^\dagger h_+^\dagger & h_+p_+p_+^\dagger h_-^\dagger & h_+p_+p_-^\dagger h_+^\dagger & h_+p_+p_-^\dagger h_-^\dagger\\
h_+p_-p_+^\dagger h_+^\dagger & h_+p_-p_+^\dagger h_-^\dagger & h_+p_-p_-^\dagger h_+^\dagger & h_+p_-p_-^\dagger h_-^\dagger\\
h_-p_+p_+^\dagger h_+^\dagger & h_-p_+p_+^\dagger h_-^\dagger & h_-p_+p_-^\dagger h_+^\dagger & h_-p_+p_-^\dagger h_-^\dagger\\
h_-p_-p_+^\dagger h_+^\dagger & h_-p_-p_+^\dagger h_-^\dagger & h_-p_-p_-^\dagger h_+^\dagger & h_-p_-p_-^\dagger h_-^\dagger
\end{bmatrix}_{k,q,r,s}(\tau)
$$

$$
=\begin{bmatrix}
p_+^\dagger h_+^\dagger h_+p_+ & p_+^\dagger h_-^\dagger h_+p_+ & p_-^\dagger h_+^\dagger h_+p_+ & p_-^\dagger h_-^\dagger h_+p_+\\
p_+^\dagger h_+^\dagger h_+p_- & p_+^\dagger h_-^\dagger h_+p_- & p_-^\dagger h_+^\dagger h_+p_- & p_-^\dagger h_-^\dagger h_+p_-\\
p_+^\dagger h_+^\dagger h_-p_+ & p_+^\dagger h_-^\dagger h_-p_+ & p_-^\dagger h_+^\dagger h_-p_+ & p_-^\dagger h_-^\dagger h_-p_+\\
p_+^\dagger h_+^\dagger h_-p_- & p_+^\dagger h_-^\dagger h_-p_- & p_-^\dagger h_+^\dagger h_-p_- & p_-^\dagger h_-^\dagger h_-p_-
\end{bmatrix}_{r,s,k,q}(\beta-\tau)
$$

$$
=\begin{bmatrix}
p_+h_+h_+^\dagger p_+^\dagger & p_+h_+h_-^\dagger p_+^\dagger & p_+h_+h_+^\dagger p_-^\dagger & p_+h_+h_-^\dagger p_-^\dagger\\
p_-h_+h_+^\dagger p_+^\dagger & p_-h_+h_-^\dagger p_+^\dagger & p_-h_+h_+^\dagger p_-^\dagger & p_-h_+h_-^\dagger p_-^\dagger\\
p_+h_-h_+^\dagger p_+^\dagger & p_+h_-h_-^\dagger p_+^\dagger & p_+h_-h_+^\dagger p_-^\dagger & p_+h_-h_-^\dagger p_-^\dagger\\
p_-h_-h_+^\dagger p_+^\dagger & p_-h_-h_-^\dagger p_+^\dagger & p_-h_-h_+^\dagger p_-^\dagger & p_-h_-h_-^\dagger p_-^\dagger
\end{bmatrix}_{q,k,s,r}(\tau)
$$

$$
C_{Q=0,S=1,S^3=+1;k,q,r,s}(\tau)=C_{Q=0,S=1,S^3=-1;r,s,k,q}{}^\top(\beta-\tau)
$$

$$
C_{Q=0,S=1,S^3=+1;k,q,r,s}(\tau)=\begin{bmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{bmatrix}C_{Q=0,S=1,S^3=+1;q,k,s,r}(\tau)\begin{bmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{bmatrix}
$$

$XF:H$

$$
\begin{aligned}
&C_{Q=0,S=1,S^3=+1;k,q,r,s}\\
&= \frac{1}{Z} tr \left[p_k h_q e^{-H\tau} h_r^\dagger p_s^\dagger e^{-H(\beta-\tau)} \right]\\
&= \frac{1}{Z} tr \left[(XF)^{-1}(XF) p_k (XF)^{-1}(XF) h_q (XF)^{-1}(XF) e^{-H\tau} (XF)^{-1}(XF) h_r^\dagger (XF)^{-1}(XF) p_s^\dagger (XF)^{-1}(XF) e^{-H(\beta-\tau)} \right]\\
&= \frac{1}{Z} tr \left[(\Sigma p)_k^\dagger (\Sigma h)_q^\dagger e^{-H\tau} (\Sigma h)_r (\Sigma p)_s e^{-H(\beta-\tau)} \right]
\end{aligned}
$$

$$
\begin{aligned}
&C_{Q=0,S=1,S^3=+1;k,q,r,s}\\
&= (XF)^{-1} \begin{bmatrix}
p_+h_+h_+^\dagger p_+^\dagger & p_+h_+h_+^\dagger p_-^\dagger & p_+h_+h_-^\dagger p_+^\dagger & p_+h_+h_-^\dagger p_-^\dagger \\
p_+h_-h_+^\dagger p_+^\dagger & p_+h_-h_+^\dagger p_-^\dagger & p_+h_-h_-^\dagger p_+^\dagger & p_+h_-h_-^\dagger p_-^\dagger \\
p_-h_+h_+^\dagger p_+^\dagger & p_-h_+h_+^\dagger p_-^\dagger & p_-h_+h_-^\dagger p_+^\dagger & p_-h_+h_-^\dagger p_-^\dagger \\
p_-h_-h_+^\dagger p_+^\dagger & p_-h_-h_+^\dagger p_-^\dagger & p_-h_-h_-^\dagger p_+^\dagger & p_-h_-h_-^\dagger p_-^\dagger
\end{bmatrix}_{k,q,r,s} (\tau)\ (XF)\\
&= \begin{bmatrix}
(\Sigma p)_+^\dagger (\Sigma h)_+^\dagger (\Sigma h)_+ (\Sigma p)_+ & (\Sigma p)_+^\dagger (\Sigma h)_+^\dagger (\Sigma h)_+ (\Sigma p)_- & (\Sigma p)_+^\dagger (\Sigma h)_+^\dagger (\Sigma h)_- (\Sigma p)_+ & (\Sigma p)_+^\dagger (\Sigma h)_+^\dagger (\Sigma h)_- (\Sigma p)_- \\
(\Sigma p)_+^\dagger (\Sigma h)_-^\dagger (\Sigma h)_+ (\Sigma p)_+ & (\Sigma p)_+^\dagger (\Sigma h)_-^\dagger (\Sigma h)_+ (\Sigma p)_- & (\Sigma p)_+^\dagger (\Sigma h)_-^\dagger (\Sigma h)_- (\Sigma p)_+ & (\Sigma p)_+^\dagger (\Sigma h)_-^\dagger (\Sigma h)_- (\Sigma p)_- \\
(\Sigma p)_-^\dagger (\Sigma h)_+^\dagger (\Sigma h)_+ (\Sigma p)_+ & (\Sigma p)_-^\dagger (\Sigma h)_+^\dagger (\Sigma h)_+ (\Sigma p)_- & (\Sigma p)_-^\dagger (\Sigma h)_+^\dagger (\Sigma h)_- (\Sigma p)_+ & (\Sigma p)_-^\dagger (\Sigma h)_+^\dagger (\Sigma h)_- (\Sigma p)_- \\
(\Sigma p)_-^\dagger (\Sigma h)_-^\dagger (\Sigma h)_+ (\Sigma p)_+ & (\Sigma p)_-^\dagger (\Sigma h)_-^\dagger (\Sigma h)_+ (\Sigma p)_- & (\Sigma p)_-^\dagger (\Sigma h)_-^\dagger (\Sigma h)_- (\Sigma p)_+ & (\Sigma p)_-^\dagger (\Sigma h)_-^\dagger (\Sigma h)_- (\Sigma p)_-
\end{bmatrix}\\
&= \begin{bmatrix}
p_-^\dagger h_-^\dagger h_- p_- & p_-^\dagger h_-^\dagger h_- p_+ & p_-^\dagger h_-^\dagger h_+ p_- & p_-^\dagger h_-^\dagger h_+ p_+ \\
p_-^\dagger h_+^\dagger h_- p_- & p_-^\dagger h_+^\dagger h_- p_+ & p_-^\dagger h_+^\dagger h_+ p_- & p_-^\dagger h_+^\dagger h_+ p_+ \\
p_+^\dagger h_-^\dagger h_- p_- & p_+^\dagger h_-^\dagger h_- p_+ & p_+^\dagger h_-^\dagger h_+ p_- & p_+^\dagger h_-^\dagger h_+ p_+ \\
p_+^\dagger h_+^\dagger h_- p_- & p_+^\dagger h_+^\dagger h_- p_+ & p_+^\dagger h_+^\dagger h_+ p_- & p_+^\dagger h_+^\dagger h_+ p_+
\end{bmatrix}_{k,q,r,s} (\tau)
\end{aligned}
$$

$$
= \begin{bmatrix}
p_-h_-h_-^\dagger p_-^\dagger & p_+h_-h_-^\dagger p_-^\dagger & p_-h_+h_-^\dagger p_-^\dagger & p_+h_+h_-^\dagger p_-^\dagger \\
p_-h_-h_+^\dagger p_-^\dagger & p_+h_-h_+^\dagger p_-^\dagger & p_-h_+h_+^\dagger p_-^\dagger & p_+h_+h_+^\dagger p_-^\dagger \\
p_-h_-h_-^\dagger p_+^\dagger & p_+h_-h_-^\dagger p_+^\dagger & p_-h_+h_-^\dagger p_+^\dagger & p_+h_+h_-^\dagger p_+^\dagger \\
p_-h_-h_+^\dagger p_+^\dagger & p_+h_-h_+^\dagger p_+^\dagger & p_-h_+h_+^\dagger p_+^\dagger & p_+h_+h_+^\dagger p_+^\dagger
\end{bmatrix}_{s,r,k,q} (\beta-\tau)
$$

$$
\begin{aligned}
&C_{Q=0,S=1,S^3=+1;k,q,r,s}(\tau)\\
&\qquad = \begin{bmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{bmatrix} C_{Q=0,S=1,S^3=-1;k,q,r,s}(\tau) \begin{bmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
&C_{Q=0,S=1,S^3=+1;k,q,r,s}(\tau)\\
&\qquad = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{bmatrix} C_{Q=0,S=1,S^3=+1;s,r,q,k}{}^\top(\beta-\tau) \begin{bmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}
\end{aligned}
$$

The table below shows the summary of all symmetries that we calculated.
For more compact form, we write

	Q	S	S^3	trafo	$kqrs$	τ
Start with	0	1	+1	1	1234	τ
trace cycl	0	1	-1	$\sigma_5 \top \sigma_5$	4321	$\beta - \tau$
I	0	1	+1	$\sigma_1 \top \sigma_1$	3412	$\beta - \tau$
	0	1	-1	$\sigma_5\sigma_1 \cdot \sigma_1\sigma_5$	2143	τ
C	0	1	-1	$\top$	3412	$\beta - \tau$
	0	1	+1	$\sigma_5 \cdot \sigma_5$	2143	τ
XF	0	1	-1	$\sigma_1 \cdot \sigma_1$	1234	τ
	0	1	+1	$\sigma_5\sigma_1 \top \sigma_1\sigma_5$	4321	$\beta - \tau$

$$\sigma_5 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

APPENDIX A

Useful information

In the appendix you usually include extra information that should be documented in your thesis, but not interrupt the flow.

The LaTeX WikiBook [12] is a useful source of information on LaTeX.

Bibliography

[1] H. Kopka and P. W. Daly, *Guide to LaTeX*, 4th ed., Addison-Wesley, 2004 (cit. on p. 1).

[2] F. Mittelbach and M. Goossens, *The LaTeX Companion*, 2nd ed., Addison-Wesley, 2004 (cit. on p. 1).

[3] Particle Data Group, K. Nakamura et al., *Review of Particle Physics*, J. Phys. G **37** (2010) 075021, URL: http://pdg.lbl.gov (cit. on p. 1).

[4] I. C. Brock, *Users Guide to Writing a Thesis in a Physics/Astronomy Institute of the Universität Bonn*, URL: http://pi.physik.uni-bonn.de/pi_only/thesis.php (visited on 01/07/2021) (cit. on p. 1).

[5] ATLAS Collaboration, *Measurement of the top quark-pair production cross section with ATLAS in pp collisions at $\sqrt{s} = 7$ TeV*, Eur. Phys. J. C **71** (2011) 1577, arXiv: 1012.1792 (cit. on p. 1).

[6] F. Halzen and A. D. Martin, *Quarks and Leptons: An Introductory Course in Modern Particle Physics*, Wiley, 1984, ISBN: 9780471887416 (cit. on p. 1).

[7] T. Loddenkötter, *Implementation of a kinematic fit of single top-quark production in association with a W boson and its application in a neural-network-based analysis in ATLAS*, BONN-IR-2012-06, PhD Thesis: University of Bonn, 2012, URL: http://hss.ulb.uni-bonn.de/diss_online (cit. on p. 1).

[8] S. Mergelmeyer, *D^*-Photoproduktion mit assoziierten Jets und Vertices bei ZEUS*, BONN-IB-2011-01, Universität Bonn, 2011, URL: http://brock.physik.uni-bonn.de/zeus_pub.php (cit. on p. 1).

[9] O. S. Brüning et al., eds., *LHC Design Report. 1. The LHC Main Ring*, CERN-2004-003-V-1, CERN-2004-003, Geneva, 2004, URL: https://cdsweb.cern.ch/record/782076 (cit. on p. 1).

[10] ATLAS Collaboration, *Determination of the muon reconstruction efficiency in ATLAS at the Z resonance in proton-proton collisons at $\sqrt{s} = 7$ TeV*, ATLAS-CONF-2011-008, CERN, 2011 (cit. on p. 1).

[11] ATLAS Collaboration, *Expected Performance of the ATLAS Experiment – Detector, Trigger and Physics*, 2009, arXiv: 0901.0512 (cit. on p. 1).

[12] *LaTeX*, URL: https://en.wikibooks.org/wiki/LaTeX (visited on 01/07/2021) (cit. on p. 13).

List of Figures

List of Tables