Characterisation and investigation of topologically nontrivial states in $\mathcal{PT}$-symmetric fermionic many-body systems

Master Thesis

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1. Introduction

The description and classification of different phases of matter are recurring problems in condensed matter physics. With the discovery of the quantum Hall effect by K. von Klitzing in 1980 [1, 2] a new field of research of previously unknown, exotic phases of matter, topological phases, has opened up. This experimental discovery was awarded with the Nobel prize five years later. In the following years a theoretical description of the quantum Hall effect using the methods of topology was established [3–11]. The forerunners of this development, Thouless, Haldane and Kosterlitz, were honoured with the Nobel prize in 2016 “for theoretical discoveries of topological phase transitions and topological phases of matter”.

As a part of mathematics, topology describes the properties of structures (or more intuitively an object, an area, or a surface) and specific, smooth deformations of these structures (like bending, stretching, twisting or other distortions). Their properties (like the orientation of their boundary, the number of holes, or the occurrence of self intersections) do not change as they are changed by such deformations, which are called homeomorphisms. If a homeomorphism that maps two structures onto one another exists, they are called topologically equivalent or homeomorphic. A set of such homeomorphic structures forms an equivalence class, which can be classified by a topological invariant. All structures from a class have all the same topological properties. The canonical example for two topological equivalent structures is a mug with a handle and a doughnut, which both possess one hole and can be homeomorphically transformed into each other. The number of holes $g$ (genus) is the topological invariant, which classifies the equivalence class containing all objects with exactly one hole. The first studies of this topic are accredited to Leonhard Euler around 1735. He is known as the originator of the famous Euler’s polyhedron formula,

\[ V - E + F = 2 - 2g , \]

which connects the number of holes of a polyhedron $g$ with its number of corners $V$ (vortices), edges $E$ and faces $F$. The right-hand side is also called Euler characteristic $\chi = 2 - 2g$. In the example of the mug and the doughnut this holds for all of their triangulations. This statements can also be formulated for the continuous objects $\mathcal{M}$ (closed two-dimensional manifolds) leading to the Gauss-Bonnet theorem,

\[ \int_{\mathcal{M}} K \cdot dA = 2\pi \chi \]
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with the Gaussian curvature $K$ of the manifold. It is about 100 years older than Euler's formula. This theorem shows that the topology (the Euler characteristic) of an object is immanently connected to its geometry (the Gaussian curvature). With the help of the Euler characteristic all objects can be organized in classes of objects with the same genus, which can be transformed into each other by bending, stretching, twisting, or other distortions.

In condensed matter physics, the energy surfaces (or bands) of solids can be treated as manifolds to which one can attribute a curvature similarly to the Gaussian curvature of a doughnut or a mug or any other object one can think of. This quantity is called Berry curvature $\mathcal{B}$ (after M. Berry [12]). If $\mathcal{B}$ is integrated over the Brillouin zone (in the style of the Gauss-Bonnet theorem), the result is found to be related to an Euler characteristic analogue called the Chern number or winding number in two respectively one-dimensional systems. This allows for the topological classification of the energy surfaces and sets the foundation for the topological band theory [13].

In the context of topological states and phases, the effects of dissipation have gained greatly in importance over the last years, as different studies have shown that dissipation can influence or even induce topological phases [14–16]. These states are of particular importance as they are topologically protected against defects and perturbations, which does not change the topology of the system. This property makes them interesting for applications like topological quantum computation [17]. Thus, a tool as dissipative effects is of special interest as it is in the position of manipulating and controlling topological states.

Two very different approaches of describing topological effects in dissipative systems can be found in literature. One approach of describing open quantum systems is based on an effective description, which uses $\mathcal{PT}$-symmetric complex potentials to induce the gain and loss of particles [18–20]. The other is based in Lindblad master equations, which uses Lindblad superoperators to describe dissipation [15, 21–24]. The relation of both approaches has never been intensively studied, and thus the validity of the effective $\mathcal{PT}$-symmetric description is one question which will be discussed in the following thesis. In this course, the case of balanced gain and loss is of major interest, as it can be easily described in the framework of $\mathcal{PT}$-symmetric complex potentials [25–30]. The influences of such potentials on topological many-body systems has been studied in lattice systems [19, 31–35] (some of them will also be part of this thesis). It has been shown that $\mathcal{PT}$-symmetric potentials are able to destroy topologically protected states which exist in analogous systems under complete isolation [31–36]. Also $\mathcal{PT}$-symmetric systems have been found in which topological states can survive [19, 20, 33–35, 37]. This has also been confirmed in experimental investigations [36, 38, 39] using optical waveguides.

In many theoretical studies the topological phases are investigated by the occurrence of edge states and their property to close an energy gap of the band structure [31, 33–35, 39]. Even tough, $\mathcal{PT}$-symmetric topological band theory is a powerful full tool for the investigation of the topology of various systems, the usage of this approach to compute topological invariants for non-Hermitian systems such as the Berry or Zak phase [12,
leads to new challenges and is in large parts restricted to systems which are analytically accessible \cite{18, 32, 42}. Especially if the eigenstates of the system are only available numerically (e.g. in the arbitrary $\mathcal{PT}$-symmetric complex potentials) there is no robust method which is able provide insight into topological properties. Such a numerical tool has been developed in course of this thesis and is presented in chapter 4. It is based on explicitly evaluating the integral of the Berry potential along closed loops in parameter space. Therefore a numerical gauge smoothing procedure has to be introduced as the occurrence of arbitrary global phases at isolated points along the loop would distort the phase relation, which allows for a numerical integration of the Berry potential.

This tool is used in the investigation of $\mathcal{PT}$-symmetric extensions of the SSH model and the Kitaev chain, as well as in the context of dissipative systems described via Lindblad master equations, for which the method of third quantisation \cite{43} is used. In essence, one can find an analogy between open quantum systems in an effective description, which uses complex $\mathcal{PT}$-symmetric potentials to describe dissipative effects and equivalent systems described by Lindblad master equations. This analogy allows for the investigation of basic properties of dissipative systems using an effective non-Hermitian theory.

**Structure of the thesis**

At first the theoretical foundations of topological aspects in quantum systems and an effective description of open systems using a non-Hermitian $\mathcal{PT}$-symmetric quantum theory are introduced in the chapters 2 and 3. The real part of the complex Zak phase \cite{40} is used as topological index, which characterises the complex band structure, and its quantisation in the $\mathcal{PT}$-unbroken parameter regime is shown.

Afterwards, the topological properties of the band structures of different modifications of the SSH model (after Su, Schrieffer and Heeger) \cite{44} and the Kitaev chain \cite{45} are investigated. These studies are build upon a numerical algorithm, which is introduced in chapter 4. It allows for the computation of the eigenvectors of a given Hamiltonian in an appropriate gauge, from which a smooth Berry potential can be obtained \cite{46}.

The results of the application of the algorithm onto the previously mentioned lattice systems can be found in section 5. The investigation reveals that topological phases exist in one-dimensional $\mathcal{PT}$-unbroken lattice systems, which can be classified by the real part of the complex Zak phase. In this course, the eigenstate corresponding to the eigenvalue with the maximal imaginary part is of special interest, because it becomes dominant in the temporal evolution. This state is called “maximal $\mathcal{PT}$-broken ground state”. The attribute “maximal $\mathcal{PT}$-broken” is also used to label states possessing the eigenvalue with a maximal imaginary part among states with a degenerate real part of the complex energy eigenvalue.

Further, a heuristic analogy is drawn between dissipative systems described in the framework of Lindblad master equations and the band theory of closed lattice systems by...
1. Introduction

identifying a Bloch Hamiltonian-like structure in the Fourier transform of the Liouvillian in chapter 6. To push the analogy further, an analogue to the Zak phase can be defined for dissipative systems. This analogy is used to investigate models which are similar to the $\mathcal{P}\mathcal{T}$-symmetric lattices in the previous part. A subsequent investigation of the steady states reveals a parallel between them and the maximal $\mathcal{P}\mathcal{T}$-broken ground states of an analogous $\mathcal{P}\mathcal{T}$-symmetric system.
2. Topological aspects in Hermitian quantum mechanics

The basis of the understanding topological aspects in quantal systems is the Berry phase, which was established by M. V. Berry in 1984 [12]. This phase characterises the geometric change of a quantum mechanical wave function under adiabatic transport in parameter space and allows for the investigation of the system’s topology when closed loops in parameter space are taken into account. Therefore the first section yields an introduction to the theory of Berry phases. Motivated by the first part of this chapter the second section provides an introduction to topological band theory.

2.1. The Berry phase

The following discussion is based on the works of Berry [12], Garrison [41] and Budich [47]. A state $|\psi(t)\rangle$ of a physical system described by the Hamiltonian $H$, which is initially prepared in an instantaneous eigenstate of the Schrödinger equation acquires a phase when transported on a curve through the system’s parameter space. This phase consists of a dynamical part caused by the unitary time evolution and a geometrical part depending on the curve on which the system is transported through parameter space.

To see this, one expands the state of the system $|\psi(t)\rangle$ in the natural basis \{ $|n(\alpha(t))\rangle : n = 1, \ldots, \dim H$ \} of the Hamiltonian $H(\alpha(t))$ at the point $\alpha(t) \in \mathbb{P}$ of the parameter space $\mathbb{P}$,

$$
|\psi(t)\rangle = \sum_{n=1}^{\dim H} c_n(t) e^{-i/\hbar \int_0^t E_n(\alpha(t')) dt'} |n(\alpha(t))\rangle , \quad (2.1)
$$

where $\alpha(t)$ describes the set of parameters of the system at time $t$ on the curve $\mathcal{C} \subset \mathbb{P}$ through parameter space. The states of the natural basis fulfil the instantaneous Schrödinger equation,

$$
H(\alpha(t)) |n(\alpha(t))\rangle = E_n(\alpha(t)) |n(\alpha(t))\rangle \quad (2.2)
$$

and the state $|\psi(\alpha(t))\rangle$ obeys the time-dependent Schrödinger equation,

$$
H(\alpha(t)) |\psi(t)\rangle = i\hbar \partial_t |\psi(t)\rangle . \quad (2.3)
$$
2. Topological aspects in Hermitian quantum mechanics

The normalisation of $|\psi(t)\rangle$ ($\langle\psi(t)|\psi(t)\rangle = 1$), and the states of the natural basis $\langle n(\alpha(t))|m(\alpha(t))\rangle = \delta_{nm}$ provide a sum formula for the coefficients $c_n(t)$,

$$\sum_{n=1}^{\dim H} |c_n(t)|^2 = 1,$$

for all $t$. To find the coefficients $c_n(t)$ one substitutes equation (2.1) into equation (2.3), where the Hamiltonian can be written in its eigenbasis, $H = \sum_m E_m |m\rangle \langle m|$ and the dependency on $\alpha(t)$ is dropped for reasons of clearness

$$H \left[ \sum_{n=1}^{\dim H} c_n(t) e^{-i/\hbar \int_0^t E_n dt'} |n\rangle \right] = i\hbar \partial_t \left[ \sum_{n=1}^{\dim H} c_n(t) e^{-i/\hbar \int_0^t E_n dt'} |n\rangle \right]$$

$$\sum_{n=1}^{\dim H} \sum_{m=1}^{\dim H} c_n(t) e^{-i/\hbar \int_0^t E_m dt'} E_m |m\rangle \langle m|n\rangle = i\hbar \sum_{n=1}^{\dim H} \left[ \dot{c}_n(t) e^{-i/\hbar \int_0^t E_n dt'} |n\rangle + c_n(t) e^{-i/\hbar \int_0^t E_n dt'} \partial_t |n\rangle \right],$$

where the dot denotes the time derivative. Projecting both sides on an instantaneous eigenstate $\langle j|$ and using their orthonormalisation one obtains a system of coupled differential equations for the coefficients $c_j(t)$

$$E_j c_j(t) = i\hbar e^{i/\hbar \int_0^t E_j dt'} \sum_{n=1}^{\dim H} \left[ \dot{c}_n(t) e^{-i/\hbar \int_0^t E_n dt'} \langle j|n\rangle + c_n(t) e^{-i/\hbar \int_0^t E_n dt'} \langle j|\partial_t|n\rangle \right]$$

$$= i\hbar \partial_t c_j(t) + E_j c_j(t) + i\hbar \sum_{n=1}^{\dim H} c_n(t) e^{-i/\hbar \int_0^t (E_n-E_j) dt'} \langle j|\partial_t|n\rangle,$$

which can be rewritten as

$$\dot{c}_j(t) + c_j(t) \langle j|\partial_t|j\rangle = \sum_{n\neq j} c_n(t) e^{-i/\hbar \int_0^t (E_n-E_j) dt'} \langle j|\partial_t|n\rangle.$$

The Berry phase can be obtained as an approximative solution of this coupled differential equation system by applying the adiabatic approximation. To do so, one introduces two parameters $s$ and $\epsilon$ fulfilling

$$t = \frac{s}{\epsilon},$$

The normalisation of $|\psi(t)\rangle$ ($\langle\psi(t)|\psi(t)\rangle = 1$), and the states of the natural basis $\langle n(\alpha(t))|m(\alpha(t))\rangle = \delta_{nm}$ provide a sum formula for the coefficients $c_n(t)$,
and takes the limit \( t \to \infty \), where \( s \) is finite and \( \epsilon \to 0 \). This transformation allows for rewriting the integral in the exponent of the right hand side of equation (2.7),

\[
\int_0^t (E_n - E_j) \, dt' = \frac{1}{\epsilon} \int_0^{s/\epsilon} (E_n - E_j) \, ds',
\]

with \( s' = \epsilon t' \). Bear in mind that the dependency on \( \alpha(t) \) was neglected in the notation. Using equation (2.9) the right hand side of equation (2.7) can be ignored in the limit \( \epsilon \to 0 \) because the exponent oscillates rapidly. The solution of the resulting uncoupled differential equation system

\[
\dot{c}_j(t) = -c_j(t) \langle j|\partial_t|j \rangle
\]

(2.10)
can be formally written as

\[
c_j(t) = c_j(0) e^{-\frac{t}{\epsilon} \langle j|\partial_t|j \rangle dt'} = c_j(0) e^{i\gamma_j(t)},
\]

(2.11)
where the Berry phase \( \gamma_j(t) \) is defined as

\[
\gamma_j(t) := i \int_0^t \langle j(\alpha(t'))|\partial_t|j(\alpha(t')) \rangle \, dt'.
\]

(2.12)
The Berry phase is the geometrical phase picked up by an instantaneous eigenstate \( |j(\alpha(t))\rangle \) of the Hamiltonian under adiabatic variation of the parameter space coordinates. The integral in equation (2.12) can be transformed to a line integral along the curve \( C \subset \mathbb{P} \) on which the system is transported through the parameter space \( \mathbb{P} \),

\[
\gamma_j(C) = i \int_C \langle j(\alpha)|\nabla_{\alpha}|j(\alpha) \rangle \cdot d\alpha.
\]

(2.13)
The normalisation of the basis states \( |j(\alpha)\rangle \) causes the Berry phase to be real valued,

\[
\langle j(\alpha)|j(\alpha) \rangle = 1 \\
\Rightarrow \nabla_{\alpha}(\langle j(\alpha)|j(\alpha) \rangle) = 0 \\
\Rightarrow \langle j(\alpha)|\nabla_{\alpha}|j(\alpha) \rangle = -(\langle j(\alpha)|\nabla_{\alpha}|j(\alpha) \rangle)^* \\
\Rightarrow \gamma_j(C) \in \mathbb{R}.
\]

(2.14)

If the system is initially prepared in a state of the natural basis \( |\psi(0)\rangle = |n(\alpha(0))\rangle \) the initial conditions can be specified as

\[
c_n(0) = 1, \\
c_m(0) = 0 \quad \text{for} \ m \neq n.
\]

(2.15)
2. Topological aspects in Hermitian quantum mechanics

Figure 2.1.: Schematic figure of the transport of an instantaneous eigenstate $|n\rangle$ on a loop $C$ in the parameter space $\mathbb{P}$ starting and ending at $\alpha(0)$. The state $|n\rangle$ picks up the phase $\gamma_n(C)$ as it travels adiabatically along the curve $C$.

The state evolving from $|n(\alpha(0))\rangle$ while the system is adiabatically transported along the curve $C$ follows from the ansatz in equation (2.1),

$$|\psi(t)\rangle = e^{-i/\hbar \int_0^t d\tau E_n(\alpha(\tau))} e^{i\gamma_n(T)} |n(\alpha(T))\rangle .$$  (2.16)

If the start and end points of the curve $C$ are identical, i.e. $\alpha(0) = \alpha(T)$, the curve $C$ is a loop in the parameter space with base point $\alpha(0)$ and period length $T$, and the line integral in equation (2.13) becomes a circuit integral. The total geometric phase change of a state initially prepared in a state of the natural basis along the loop $C$ is

$$\gamma_n(C) = i \oint_C \langle n(\alpha) | \nabla_\alpha | n(\alpha) \rangle \cdot d\alpha .$$  (2.17)

The transport of a state $|n\rangle$ through the parameter space is illustrated in figure 2.1.

The integrand of equation (2.17) depends on the gauge of the eigenvectors $|n(\alpha)\rangle$ and is called Berry connection, denoted as

$$A_n(\alpha) := i \langle n(\alpha) | \nabla_\alpha | n(\alpha) \rangle .$$  (2.18)

The state $|n'(\alpha)\rangle$ obtained by a local $U(1)$ phase transformation from the state $|n(\alpha)\rangle$

$$|n'(\alpha(t))\rangle = |n(\alpha(t))\rangle e^{i\varphi_n(\alpha(t))}$$  (2.19)

is also a solution of equation (2.2) and leads to a transformed Berry connection

$$A'_n(\alpha) = i \langle n'(\alpha) | \nabla_\alpha | n'(\alpha) \rangle = A_n(\alpha) - \nabla_\alpha \varphi_n(\alpha(t)) .$$  (2.20)

The berry curvature is obtained from the Berry connection and is an anti-symmetric second-rank tensor which is defined as

$$B_{n,i,j}(\alpha) = \partial_{\alpha_i} A_{n,j}(\alpha) - \partial_{\alpha_j} A_{n,i}(\alpha) ,$$  (2.21)
or in three dimensions simply as the curl of $A$. This relation is just for matters of completeness and will not be used in the following.

The Berry phase following from $|n'(\alpha)\rangle$ can be expressed in terms of the Berry connection of $|n(\alpha)\rangle$,

$$
\gamma'_n(C) = \oint_C A'_n(\alpha) \cdot d\alpha
$$

$$
= \oint_C \left( A_n(\alpha) - \nabla_\alpha \varphi_n(\alpha(t)) \right) \cdot d\alpha
$$

$$
= \gamma_n(C) - \oint_C \nabla_\alpha \varphi_n(\alpha(t)) \cdot d\alpha
$$

$$
= \gamma_n(C) - \left( \varphi_n(\alpha(T)) - \varphi_n(\alpha(0)) \right)
$$

(2.22)

where in the last step the fundamental theorem of calculus for line integrals was used to calculate the circuit integral of the gradient of the gauge function. Since the basis has to be single valued in parameter space, the states $|n(\alpha)\rangle$ and $|n'(\alpha)\rangle$ have to be identical (modulo a phase factor of $\exp(z 2\pi)$) for every point $\alpha$ such that

$$
\varphi_n(\alpha(t)) = \varphi_n(\alpha(t + T)) + z 2\pi
$$

(2.23)

with $z \in \mathbb{Z}$. This causes the Berry phase to be defined only up to a phase shift of $2\pi$ as equation (2.22) becomes

$$
\gamma'_n(C) = \gamma_n(C) + z 2\pi.
$$

(2.24)

Aharonov et al. [48] pointed out that the Berry Phase is only a limiting case of a more general geometric phase associated with a closed curve in the projective Hilbert space.

Another interpretation of the Berry phase can be obtained from equation (2.12), from which one can derive a relation to the area enclosed by the components of the instantaneous eigenstates $|n\rangle$ in the complex plane while the system is transported along the loop $C$ in parameter space. To this end one writes the eigenstate as

$$
|n(\alpha(t))\rangle = \left( n_1(\alpha(t)), ..., n_i(\alpha(t)), ..., n_d(\alpha(t)) \right)^T
$$

(2.25)

with $d = \dim H$, the components of the eigenstate $n_i = x_i + iy_i \in \mathbb{C}$ and $x_i, y_i \in \mathbb{R}$. The line on which the component $n_i$ moves in the complex plane as the system is transported on the loop $C$ through the parameter space is denoted as $C_i$. Then the Berry phase can
be expressed as

$$
\gamma_n(C) = i \int_0^T \langle n(\alpha(t))|\partial_t|n(\alpha(t)) \rangle \, dt'
$$

$$
= \sum_{i=1}^d i \oint n^*_i \, dn_i
$$

$$
= \sum_{i=1}^d i \oint (x_i \, dx_i + x_i \, dy_i - y_i \, dx_i - y_i \, dy_i)
$$

$$
= \sum_{i=1}^d i \oint (x_i \, dy_i - y_i \, dx_i)
$$

$$
= -2 \sum_{i=1}^d \text{area}(\mathcal{D}_i),
$$

(2.26)

where at time $t = 0$ and $t = T$ the system is in the base point of the loop $C$, which causes

$$
\oint_{\mathcal{C}_i} x_i \, dx_i = \oint_{\mathcal{C}_i} y_i \, dy_i = 0.
$$

(2.27)

To obtain the result Green’s theorem was applied in the last step to identify the area of the surface $\mathcal{D}_i$ enclosed by the loop $\mathcal{C}_i = \partial \mathcal{D}_i$ in the complex plane. The Berry phase corresponding to the eigenstate $|n\rangle$ is therefore the sum of the areas enclosed by each component, as the system is transported on the loop $C$ through the parameter space, multiplied by $-2$.

### 2.1.1. The Berry phase in discrete parameter space

In the case of a discrete parameter space the loop in parameter space is a set of neighbouring points $C = (\alpha_1, ..., \alpha_j, ..., \alpha_M = \alpha_1)$. In the following the states of the instantaneous basis corresponding to a point $\alpha_j$ are subscripted by $j$. In this case the Berry phase takes the form

$$
\gamma_n = i \ln \left( \prod_{j=0}^{M-1} \langle n_j|n_{j+1} \rangle \right),
$$

(2.28)

as shown by Yaschenko et al. [49]. This has an illustrative interpretation. The phase factor

$$
e^{i\gamma_n} = \prod_{j=0}^{M-1} \langle n_j|n_{j+1} \rangle = \prod_{j=0}^{M-1} e^{i\gamma_{n,j,j+1}}
$$

(2.29)
2.2. Topological band theory

Figure 2.2.: Illustration of a discrete loop $C$ in parameter space. Here the dependency on $\alpha$ was dropped in the notation for matters of clarity. The states pick up a phase for every step in the discretised parameter space.

gathered up by a state transported through the parameter space is the product of the projections of neighbouring states on each other. This statement is illustrated in figure 3.1. In this process it is important to identify the first and the last state at the point $\alpha_1 = \alpha_M$ in parameter space. The discrete formulation of the Berry phase is immanently gauge invariant, because a local $U(1)$ gauge transformation $\exp(i\varphi_{n,j})$ of the state $|n_j\rangle$ appears twice in the product of scalar products of neighbouring states (cf. (2.28)) once as $\exp(i\varphi_{n,j})$ and once complex conjugated. Thus all phase factors $\exp(i\varphi_{n,j})$ cancel out in the product.

2.2. Topological band theory

In the second part of this thesis topological phases of one-dimensional lattice systems are investigated by calculating the Zak phase of the eigenstates $|j\rangle$ of the Bloch Hamiltonian $\mathcal{H}$

$$\gamma_j = i \oint_{\mathcal{BZ}} \langle j | \partial_k | j \rangle \, dk , \quad (2.30)$$

which is the Berry phase picked up by the system when it is transported through the first Brillouin zone $\mathcal{BZ} \subset \mathbb{P}$ (which acts as loop in parameter space $\mathbb{P}$).

To introduce the topic the generic fermionic Hamiltonian

$$H = \sum_{n,m=1}^{N} c_n^\dagger H_{n,m} c_m $$ \hspace{1cm} (2.31)

is discussed in the following. The Hamiltonian $H$ describes a one-dimensional lattice of $N$ lattice sites with hopping amplitudes $H_{i,j}$ for $i \neq j$ and real on-site potentials $H_{i,i}$. Let the Hamiltonian be translationally invariant, with unit cells containing $M$ lattice sites. By making use of this translational symmetry and introducing the Fourier representation of the annihilation operator,

$$c_n = \frac{1}{\sqrt{N/M}} \sum_{k=-\pi}^{\pi} c_k e^{-i kn} , \quad (2.32)$$
one obtains
\[ H = \sum_{k=-\pi}^{\pi} \sum_{i,j=1}^{M} c_{k,i}^\dagger H_{i,j} c_{k,j} \] (2.33)
with the Bloch Hamiltonian of the system \( \mathcal{H} \).

An alternative notation for the Fourier transform can be found in appendix A. This procedure is used to calculate the Bloch Hamiltonian of lattice systems exhibiting unit cells with more lattice sites later on in this thesis.

A general \((2 \times 2)\)-Bloch Hamiltonian can be decomposed into the Pauli matrices,
\[
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\] (2.34)
and the \((2 \times 2)\)-identity matrix denoted as \( \sigma_0 \),
\[
\mathcal{H} = n_{\alpha,0}(k)\sigma_0 + n_{\alpha}(k) \cdot \sigma,
\] (2.35)
where the eigenvalues are given by \( E_{\pm} = n_{\alpha,0} \pm |n_{\alpha}(k)| \), the vector of Pauli matrices is denoted as \( \sigma \) and the vector \( n_{\alpha}(k) \) depends on \( k \). All other variables of the parameter space are denoted by \( \alpha \in P \setminus \mathbb{Z} \) and are held constant. If an energy shift is applied such that
\[
\tilde{\mathcal{H}} = n_{\alpha}(k) \cdot \sigma,
\] (2.36)
and the normalised and energy shifted Hamiltonian defined by
\[
\hat{\mathcal{H}} = \frac{n_{\alpha}(k)}{|n_{\alpha}(k)|} \cdot \sigma = \hat{n}_{\alpha}(k) \cdot \sigma
\] (2.37)
is investigated some general statements concerning the topology of the system can be given.

The one-dimensional Brillouin zone \( \mathcal{BZ} \) is isomorphic to the unit circle \( \mathcal{BZ} \cong S^1 \). The family \( \{\hat{n}_{\alpha}\}_{\alpha \in P \setminus \mathbb{Z}} \) of mappings
\[
\hat{n}_{\alpha} : \mathcal{BZ} \rightarrow S^2, \quad k \mapsto n_{\alpha}(k)
\] (2.38)
map a circle to the unit sphere \( S^2 \). Therefore the homotopy classes of the mappings \( \{\hat{n}_{\alpha}\}_{\alpha \in P \setminus \mathcal{BZ}} \) form the fundamental group \( \pi_1(S^2) \) which is isomorphic to the trivial group \([50]\). Hence systems with Bloch Hamiltonians characterised by such coefficient vectors cannot exhibit topologically nontrivial phases.

If the image of the mappings \( n_{\alpha} \) is restricted on a circle \( S^1 \subset S^2 \) such that the mapping \( n_{\alpha} \) is characterised by
\[
\hat{n}_{\alpha} : \mathcal{BZ} \rightarrow S^1, \quad k \mapsto n_{\alpha}(k)
\] (2.39)
the underlying Hamiltonian can possess topological nontrivial phases as the fundamental group formed by the homotopy classes of the mappings \( \{ \hat{n}_\alpha \}_{\alpha \in \mathbb{P} \setminus \mathbb{BZ}} \) is \( \pi_1(S^1) \cong \mathbb{Z} \), which is nontrivial \([50]\).

Thus a two-band model can only show topologically nontrivial behaviour if the vector \( \mathbf{n}_\alpha \) characterising the Hamiltonian is restricted to a loop which is isomorphic to \( S^1 \). Such restrictions can be caused by a chiral symmetry \( \Lambda \) of the system transferring over to the Bloch Hamiltonian,

\[
\{ \Lambda, \mathcal{H} \} = 0 .
\]

(2.40)
The chiral symmetry can be decomposed into the Pauli matrices

\[
\Lambda = a_0 \sigma_0 + \mathbf{a} \cdot \mathbf{\sigma} ,
\]

(2.41)
which fulfil the commutation relations

\[
[\sigma_i, \sigma_j] = 2i \epsilon_{ijk} \sigma_k, \quad \{ \sigma_i, \sigma_j \} = 2 \delta_{ij} \sigma_0 .
\]

(2.42)
The Bloch Hamiltonian of a two band system possessing a chiral symmetry is characterised by a vector \( \mathbf{n}_\alpha(k) \) which is restricted to a plane with a normal vector \( \mathbf{a} \). This can be seen from the fact that \( \Lambda \) is a chiral symmetry of the system

\[
\{ \Lambda, \mathcal{H} \} = 0 ,
\]

\[
\{ \mathbf{a} \cdot \mathbf{\sigma}, \mathbf{n}_\alpha(k) \cdot \mathbf{\sigma} \} = 0 ,
\]

\[
\sum_{i,j=1}^{3} \{ a_i \sigma_i, n_{\alpha,j}(k) \sigma_j \} = 0 ,
\]

\[
2 \sum_{i,j=1}^{3} a_i n_{\alpha,j}(k) \delta_{ij} \sigma_0 = 0 ,
\]

\[
2 \sigma_0 \sum_{i=1}^{3} a_i n_{\alpha,i}(k) = 0 ,
\]

\[
\implies \mathbf{a} \perp \mathbf{n}_\alpha(k) .
\]

(2.43)
Without loss of generality one can consider the case \( \mathbf{a} = e_3 = e_z \) and perform a rotation of the basis if other vectors \( \mathbf{a} \) arise. In this case the component \( n_{\alpha,3} \) of the vector \( \mathbf{n}_\alpha \) vanishes. The bulk winding number \( \nu \in \mathbb{Z} \) is a topological invariant of the system, which counts the number of times the vector \( \mathbf{n}_\alpha(k) \) winds around the origin in the plane perpendicular to \( \mathbf{a} \) as \( k \) is varied from \( -\pi \) to \( \pi \),

\[
\nu_\alpha = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathbf{n}_\alpha(k) \times \partial_k \mathbf{n}_\alpha(k) \, dk
\]

\[
= \frac{1}{2\pi} \int_{-\pi}^{\pi} \left[ n_{\alpha,1} \partial_k n_{\alpha,2} - n_{\alpha,2} \partial_k n_{\alpha,1} \right] \, dk ,
\]

(2.44)
2. Topological aspects in Hermitian quantum mechanics

Figure 2.3.: Schematic illustration of the energy bands and the vector $\mathbf{n}$ characterising the Bloch Hamiltonian in the topologically different phases of a two-band model (SSH model). The dispersion relations in figure (a) and (c) are the same, whereas the winding number $\nu$ is different. In (b) the winding number is undefined as the vector passes the origin and the band gap vanishes.

and can be associated with the Zak phase. A possible pair of normalised eigenstates $|j_{\alpha,\pm}\rangle$ of a Hamiltonian characterized by equation (2.35) under the restriction $n_{\alpha,0} = n_{\alpha,3} = 0$ is

$$|j_{\pm}\rangle = \frac{1}{\sqrt{2}} \left( \frac{n_{\alpha,1} - in_{\alpha,2}}{\pm|\mathbf{n}_\alpha|} \right)$$

(2.45)

with eigenvalues $E_{\alpha,\pm} = \pm |\mathbf{n}_\alpha|$. The Zak phase (cf. equation (2.30)) is then given by [51]

$$\gamma_{\alpha,\pm} = \frac{i}{2} \oint_{BZ} \frac{\partial_k}{\pm \sqrt{n_{\alpha,1}^2 + n_{\alpha,2}^2}} \frac{n_{\alpha,1} - in_{\alpha,2}}{\pm \sqrt{n_{\alpha,1}^2 + n_{\alpha,2}^2}} \, dk$$

$$= \frac{1}{2} \oint_{BZ} \frac{n_{\alpha,1} \partial_k n_{\alpha,2} - n_{\alpha,2} \partial_k n_{\alpha,1}}{n_{\alpha,1}^2 + n_{\alpha,2}^2} \, dk$$

(2.46)

$$= \pi \nu ,$$

where the winding number is an integer indicating different topological phases and the Zak phase is a real valued number taking only the values 0 or $\pi$ because the Berry phase is defined up to multiples of $2\pi$. A detailed calculation can be found in appendix B. The relation between the winding number and the Zak phase exemplifies an important fact. The Zak phase can only change if the gap between the energy bands closes. Thus a necessary condition for a topological phase transition between two phases characterised by different Zak phases is a touching of the energy bands corresponding to the eigenstates involved in the phase transition. This is illustrated in figure 2.3 where the energy bands and the vector $\mathbf{n}_\alpha$ are depicted for three different sets of parameters $\alpha$. The topologically trivial and nontrivial phases correspond to a gapped dispersion relation, where the
2.2. Topological band theory

Figure 2.4.: Schematic sketch of a section of the SSH model with tunnelling amplitudes $t_-$ and $t_+$. The lattice can be divided into two sublattices labelled with A and B. A unit cell consists of an A site and a B site.

winding number is either 0 or 1. The phase transition occurs at a set of parameters $\alpha$ for which the dispersion relation is gapless and the vector $n_\alpha$ runs through the origin (cf. figure 2.3 (b)).

The ground state of one-dimensional non-interacting lattice models can be topologically classified by the sum of the Zak phases $\gamma$ over all occupied bands (bands with negative energy) [52].

2.2.1. An example – the SSH model

The most straightforward lattice model, which is able to show topological properties is a one-dimensional lattice with two different tunnelling amplitudes $t_-$ and $t_+$ and no on-site potentials (cf. figure 2.4). This model was introduced by Su, Schrieffer and Hegger in 1979 and is therefore named SSH-model. The matrix

\[
H = \begin{pmatrix}
0 & t_- & 0 & t_+ & t_- & 0 & t_+ & \cdots \\
t_- & 0 & t_+ & \cdots \\
0 & t_+ & 0 & \cdots \\
\cdots & 0 & t_+ & 0 & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
t_+ & \cdots & \cdots & t_- & \cdots & \cdots & \cdots & \cdots \\
t_- & \cdots & \cdots & t_+ & \cdots & \cdots & \cdots & \cdots \\
\end{pmatrix}
\]

inserted into equation (2.31) characterizes the bulk of the SSH-model with two lattice sites per unit cell and periodic boundary conditions. A Fourier transform can be applied following the steps shown in appendix A leading to a ($2 \times 2$)-Bloch Hamiltonian of the form

\[
H = \begin{pmatrix}
0 & t_- + t_+ e^{i k} \\
t_- e^{-i k} & t_- + t_+ e^{i k} \\
\end{pmatrix}
= (t_- + t_+ \cos(k)) \sigma_1 - t_+ \sin(k) \sigma_2,
\]

with eigenvalues $E_\pm(k) = \pm \sqrt{(t_- + t_+ \cos(k))^2 + (t_+ \sin(k))^2}$.

There are two topologically distinct phases. The case $t_- > t_+$ corresponds to the topologically trivial phase with no edge states. It is depicted in figure 2.5 (a). The lattice sites at the edges are coupled with strong hopping amplitudes to the neighbouring sites, which is why an excitation at the edge tunnels into the bulk of the system. This case
2. Topological aspects in Hermitian quantum mechanics

\[ t_- - t_+ + t_- - t_+ - t_- + t_+ \]

belongs to the situation illustrated in figure 2.3 (a), in which the winding number is zero. In the topologically nontrivial case the tunnelling amplitudes fulfil \( t_+ > t_- \), such that the lattice sites at the edges are weakly coupled to the rest of the system. In this case the occupation of an edge state localized at one of the edges of the lattice does not require energy and thus they are also called zero energy modes. The topologically nontrivial phase corresponds to a winding number of one, shown schematically in figure 2.3 (c). The transition between these two phases occurs when the bulk band gap vanishes, which happens when the tunnelling amplitudes are the same as in this case the energies are equal to zero for \( k = \pm \pi \). At the phase transition the winding number is undefined. The phase transition corresponds to figure 2.3 (b).

2.3. Connection to the generalized winding number

The winding number can be generalized to systems with interacting particles [53, 54]. In case of systems with only next neighbour hopping the Bloch Hamiltonian is motivation for this generalization. Therefore one applies generalized boundary conditions to the lattice

\[ |\psi(x_i + L)\rangle = e^{i\phi} |\psi(x_i)\rangle , \]

where \( x_i \) is the coordinate of the \( i \)-th lattice site and \( L \) the length of the lattice. This can be realised by multiplying the tunnelling amplitudes, which connect neighbouring unit cells by a phase factor \( e^{i\phi} \). This results in analogous phase factors of the corresponding matrix elements of the Hamiltonian. In the one particle picture the resulting matrix representation of the Hamiltonian of the lattice system is equivalent the Bloch Hamiltonian for \( k \rightarrow \phi \). One sets up the matrix representation in the many-particle basis and computes the phase which is picked up by the ground state when the phase \( \phi \) is varied from \( -\pi \) to \( \pi \).
3. Biorthogonal quantum mechanics

This chapter contains an introduction to the framework of non-Hermitian $\mathcal{PT}$-symmetric operators in quantum mechanics. In this thesis $\mathcal{PT}$-symmetric quantum mechanics is used as an effective theory of open quantum systems. In this scope $\mathcal{PT}$-symmetric Hamiltonians occur, which have a biorthogonal basis of left and right handed eigenstates. These eigenstates are not orthogonal in the sense of Hermitian quantum mechanics but form a biorthogonal basis. This allows for the definition of a complex Berry phase [41], which will be introduced in the second part of this chapter. Further it is explicitly shown that the real part of the complex Berry phase is quantised in the $\mathcal{PT}$-unbroken parameter regime of a $\mathcal{PT}$-symmetric system.

3.1. $\mathcal{PT}$ symmetry

A detailed introduction to $\mathcal{PT}$ symmetry can be found in the works of Bender et al. [25, 55]. A system is $\mathcal{PT}$-symmetric if the combination of the parity and the time inversion operator commutes with the Hamiltonian of the system $\hat{H}$, i.e.

$$[\hat{H}, \mathcal{PT}] = 0.$$ (3.1)

The parity operator $\mathcal{P}$ and the time inversion operator $\mathcal{T}$ are defined by their commutation relations with the position and the momentum operator $x$ and $p$,

$$\{\mathcal{P}, x\} = 0, \quad \{\mathcal{P}, p\} = 0, \quad [\mathcal{T}, x] = 0, \quad [\mathcal{T}, p] = 0, \quad [\mathcal{T}, i] = 0.$$ (3.2)

Both, $\mathcal{P}$ and $\mathcal{T}$ are their own inverse. The parity operator is linear, whereas the time inversion operator acts as a complex conjugation and is therefore antilinear. Hence the operator $\mathcal{PT}$ is antilinear, own inverse and fulfils the commutation relations

$$\{\mathcal{PT}, x\} = 0, \quad [\mathcal{PT}, p] = 0, \quad \{\mathcal{PT}, i\} = 0.$$ (3.4)

All possible eigenvalues of $\mathcal{PT}$ form the unit circle $S^1 = \{e^{i\varphi} | \varphi \in \mathbb{R}\}$,

$$\mathbb{I} |u\rangle = (\mathcal{PT})^2 |u\rangle = \mathcal{PT}(\lambda |u\rangle) = \lambda^* \lambda |u\rangle = |\lambda|^2 |u\rangle \implies \lambda = e^{i\varphi},$$ (3.5)
3. Biorthogonal quantum mechanics

where $I$ is the identity operator. An eigenstate $|u\rangle$ of the $\mathcal{PT}$ operator is called exact $\mathcal{PT}$-symmetric if it is an eigenstate with the eigenvalue $\tilde{\lambda} = 1$. A state can always be transformed to an exact $\mathcal{PT}$-symmetric state by a $U(1)$ phase transformation,

$$\mathcal{PT}(\lambda |u\rangle) = \lambda^* \lambda |u\rangle = |\lambda|^2 |u\rangle = |u\rangle,$$

which means that if $\lambda$ is the eigenvalue of $\mathcal{PT}$ corresponding to $|u\rangle$, the state $\lambda |u\rangle$ has the eigenvalue $\tilde{\lambda} = 1$.

In the case of $|v_n\rangle$ being an eigenstate of a $\mathcal{PT}$-symmetric Hamiltonian with eigenvalue $E_n$ one finds $\mathcal{PT}|v_n\rangle$ to be an eigenstate of $H$ with eigenvalue $E_n^*$,

$$H|v_n\rangle = E_n |v_n\rangle$$

$$\mathcal{PT}H|v_n\rangle = \mathcal{PT}E_n |v_n\rangle$$

$$H\mathcal{PT}|v_n\rangle = E_n^* \mathcal{PT}|v_n\rangle.$$

If $|v_n\rangle$ is in addition an eigenstate of the $\mathcal{PT}$ operator with eigenvalue $\lambda_n \in S^1$, the eigenvalue $E_n$ is real-valued,

$$H \mathcal{PT}|v_n\rangle = E_n^* \mathcal{PT}|v_n\rangle$$

$$\lambda_n E_n |v_n\rangle = \lambda_n H|v_n\rangle = H \lambda_n |v_n\rangle = E_n^* \lambda_n |v_n\rangle = \lambda_n E_n^* |v_n\rangle$$

$$\implies E_n \in \mathbb{R}.$$

Given the case that all eigenstates of $H$ are also eigenstates of $\mathcal{PT}$ the Hamiltonian has unbroken $\mathcal{PT}$ symmetry, otherwise the $\mathcal{PT}$ symmetry of $H$ is broken [55]. These two terms are used in the following also for single states of an Hamiltonian. A state is called $\mathcal{PT}$-unbroken if its eigenvalue is real-valued and $\mathcal{PT}$-broken in case of complex eigenvalues. Thus it is possible to find $\mathcal{PT}$-unbroken states in the $\mathcal{PT}$-broken parameter regime of an Hamiltonian.

In the following a simple consequence of $\mathcal{PT}$-symmetric quantum mechanics is shown at the example of a particle in a $\mathcal{PT}$-symmetric complex potential in one dimension. The Hamiltonian of the system shall be given by

$$H = \frac{p^2}{2m} + V(x).$$

To derive a continuity equation for this system one starts with the time-dependent Schrödinger equation,

$$i\hbar \partial_t \psi(x,t) = -\frac{\hbar^2}{2m} \partial_x^2 \psi(x,t) + V(x) \psi(x,t),$$

and finds the analogous equation for $\psi^*(-x,t)$ by complex conjugation and inversion,

$$-i\hbar \partial_t \psi^*(x,t) = -\frac{\hbar^2}{2m} \partial_x^2 \psi^*(x,t) + V^*(x) \psi^*(x,t).$$
where the complex potential has to fulfill $V(x) = V^*(-x)$ to ensure $\mathcal{PT}$ symmetry. By constructing the time derivative of the probability density function and using equations (3.10) and (3.11) one obtains a generalized continuity equation,

$$
\partial_t \rho(x,t) = \partial_t \left( \psi^*(x,t) \psi(x,t) \right) \\
= \psi(x,t) \partial_t \psi^*(x,t) + \psi^*(x,t) \partial_t \psi(x,t) \\
= -\frac{\psi(x,t)}{i\hbar} \left[ -\frac{\hbar^2}{2m} \partial_x^2 \psi^*(x,t) + V^*(x) \psi^*(x,t) \right] \\
+ \frac{\psi^*(x,t)}{i\hbar} \left[ -\frac{\hbar^2}{2m} \partial_x^2 \psi(x,t) + V(x) \psi(x,t) \right] \\
= \frac{1}{i\hbar} \left[ \frac{\hbar^2}{2m} \left( \psi(x,t) \partial_x^2 \psi^*(x,t) - \psi^*(x,t) \partial_x^2 \psi(x,t) \right) \\
+ 2i \text{Im}(V(x)) \psi^*(x,t) \psi(x,t) \right] \\
= -\partial_x j(x,t) + \frac{2}{\hbar} \text{Im}(V(x)) \\
$$

(3.12)

with the probability current density $j = i\hbar/2m \left( \psi \partial_x \psi^* - \psi^* \partial_x \psi \right)$. This simple example shows that a negative (resp. a positive) imaginary part of $V(x)$ acts as a sink (resp. a source) of the probability density. Thus $\mathcal{PT}$-symmetric potentials will be used later on to effectively describe open lattice systems.

### 3.2. The complex Berry phase

In this thesis $\mathcal{PT}$-symmetric Hamiltonians $H \neq H^\dagger$ fulfilling the left and right hand versions of the Schrödinger equation,

$$
\langle \chi_n | H = E_n \langle \chi_n | , \quad H | \phi_n \rangle = E_n | \phi_n \rangle \\
H^\dagger | \chi_n \rangle = E_n^* | \chi_n \rangle , \quad \langle \phi_n | H^\dagger = E_n^* \langle \phi_n | \\
$$

(3.13)

are investigated. For simplicity the eigenvalues $E_n$ are considered to be non-degenerate in the following. The left eigenstates $\langle \chi_n |$ of such Hamiltonians are different from the adjoint right eigenstates $| \phi_n \rangle$. Both sets of vectors $\{ \langle \chi_n | \}$ and $\{ | \phi_n \rangle \}$ are in general not orthogonal but form a biorthogonal basis with the norm convention [56]

$$
\langle \chi_n | \phi_m \rangle = \delta_{nm} . \\
$$

(3.14)

An arbitrary right hand state $| \psi(t) \rangle$ can be expanded in the left instantaneous eigenstates of the biorthogonal basis, the same holds for the biorthogonal partner $\langle \xi(t) |$ [41],

$$
| \xi(t) \rangle = \sum_n c_n^* e^{i/\hbar \int_0^t E_n^*(\alpha(t')) dt'} \langle \chi_n | , \quad | \psi(t) \rangle = \sum_n c_n e^{-i/\hbar \int_0^t E_n(\alpha(t')) dt'} | \phi_n \rangle . \\
$$

(3.15)
3. Biorthogonal quantum mechanics

A detailed introduction into the main features of biorthogonal quantum mechanics can be found in [56]. The derivation of the Berry phase shown in section 2.1 can be generalized to non-Hermitian Hamiltonians with a biorthogonal basis as shown in [41] and [57] by substituting the instantaneous eigenstates in the Hermitian case by the left and right hand versions. One finds a coupled differential equation system analogous to equation (2.7) for the coefficients $c_n(t)$ of an arbitrary state $|\psi(t)\rangle$ with a vector $\alpha \in \mathbb{P}$ in parameter space $\mathbb{P}$,

$$\dot{c}_j(t) + c_j(t) \langle \chi_j | \partial_t | \phi_j \rangle = \sum_{n \neq j} c_n(t) e^{-i/\hbar} \int_0^t (E_n - E_j) d\tau \langle \chi_j | \partial_t | \phi_n \rangle .$$  \hspace{1cm} (3.16)

If the adiabatic theorem is applicable this leads to an analogous expression for the Berry phase for non-Hermitian systems [41],

$$\gamma_n = i \oint_C \langle \chi_n | \nabla_\alpha | \phi_n \rangle \cdot d\alpha .$$  \hspace{1cm} (3.17)

This is the definition of the complex Berry phase $\gamma_n \in \mathbb{C}$. The imaginary part of the complex Berry phase causes dissipative effects, which occur due to the adiabatic transportation of the system through the parameter space. The application of the adiabatic approximation is not as straightforward as in the Hermitian case [57]. In general the energies $E_n \in \mathbb{C}$ are complex and the argument of the Hermitian case applies only to the parameter regime of unbroken $\mathcal{PT}$ symmetry, where $E_n \in \mathbb{R}$. In the case of complex energies the right hand side of equation (3.16) cannot be neglected, as the summands grow exponentially for $\text{Im}(E_n - E_j) > 0$. Hence the full system of differential equations has to be solved and the phase of a certain eigenstate depends generally on all other states of the biorthogonal basis. However, the complex Berry phase is well defined in the $\mathcal{PT}$-unbroken case, for which the following part will provide an argument for the quantisation of the real part of the complex Berry phase, such that it can be used as topological invariant similarly to the Hermitian case, and thus allows for the generalisation of the topological band theory on $\mathcal{PT}$-symmetric systems.

3.2.1. Quantisation of the real part of the complex Berry phase

In the presence of an antiunitary symmetry the Berry phase of Hermitian systems is quantised as shown in the work of Hatsugai [58]. The argument for the Hermitian case is transferable to non-Hermitian $\mathcal{PT}$-symmetric systems, where the real part of the complex Berry phase takes quantised values in the $\mathcal{PT}$-unbroken regime. $\mathcal{PT}$ symmetry takes on the role of the antiunitary symmetry, which is necessary for the quantisation. To see this, one takes the biorthogonal basis $\{ \langle \chi_n | , | \phi_n \rangle \}$ of a $\mathcal{PT}$-symmetric Hamiltonian $H$ consisting of the left and right hand eigenstates of the Schrödinger equation (3.13), where $E_n$ is the eigenvalue corresponding to the pair of basis vectors $\langle \chi_n |$ and $| \phi_n \rangle$. The
states of the biorthogonal basis are chosen to fulfil the normalisation convention defined by equation (3.14). The complex Berry connection $A_n$ is given by [41]

$$A_n = i \langle \chi_n | d | \phi_n \rangle$$

(3.18)

with the exterior derivative $d$. By expressing the eigenstates in a Cartesian basis,

$$\langle \chi_n | = \sum_{j=1}^{\text{dim} H} b_{nj} \langle e_j |$$

$$| \phi_n \rangle = \sum_{j=1}^{\text{dim} H} c_{nj} | e_j \rangle$$

(3.19)

and inserting this relations to (3.18) one finds

$$A_n = i \sum_{i,j}^{\text{dim} H} b_{ni} d c_{nj} \langle e_i | e_j \rangle = i \sum_{i=1}^{\text{dim} H} b_{ni} d c_{ni}$$

(3.20)

as expression for the complex Berry connection, where the Kronecker delta $\delta_{ij} = \langle e_i | e_j \rangle$ was used to obtain the result. To establish a relation between $A_n$ and $A^{PT}_n$ corresponding to the $\mathcal{PT}$-symmetric partners of $\langle \chi_n |$ and $| \phi_n \rangle$ one applies the $\mathcal{PT}$ operator to the eigenstates,

$$\langle \chi^{PT}_n | = \sum_{j=1}^{\text{dim} H} b^*_{nj} \langle e_j |$$

$$| \phi^{PT}_n \rangle = \sum_{j=1}^{\text{dim} H} c^*_{nj} | e_j \rangle$$

(3.21)

with the notation $\mathcal{PT} \langle \chi_n | = \langle \chi^{PT}_n |$ and $\mathcal{PT} | \phi_n \rangle = | \phi^{PT}_n \rangle$ and finds

$$A^{PT}_n = i \sum_{i,j}^{\text{dim} H} b^*_{ni} d c^*_{nj} \langle e_i | e_j \rangle = i \sum_{i=1}^{\text{dim} H} b^*_{ni} d c^*_{ni} = -A^*_n$$

(3.22)

by inserting equation (3.21) into equation (3.18). A relation for the complex Berry phase and the complex Berry phase of the $\mathcal{PT}$ transformed states can be obtained from equation (3.22) by integrating the Berry connection over a loop $C$ in the parameter space,

$$\gamma_n = \oint_C A_n = - \oint_C A^{PT*}_n = - \gamma^{PT*}_n.$$  

(3.23)

Further, a second relation between $A_n$ and $A^{PT}_n$ can be obtained from equation (3.13) in the $\mathcal{PT}$-unbroken regime. The $\mathcal{PT}$-symmetric Hamiltonian fulfils the commutation relation $[H, \mathcal{PT}] = 0$. By applying the $\mathcal{PT}$ operator on the right hand Schrödinger equation and using the $\mathcal{PT}$ symmetry of $H$ one finds in the $\mathcal{PT}$-unbroken regime with real eigenvalues $E_n = E^*_n$,

$$H | \phi_n \rangle = E_n | \phi_n \rangle$$

$$\mathcal{PT} (H | \phi_n \rangle) = \mathcal{PT} (E_n | \phi_n \rangle)$$

$$H | \phi^{PT}_n \rangle = E^*_n | \phi^{PT}_n \rangle$$

$$H | \phi^{PT}_n \rangle = E_n | \phi^{PT}_n \rangle.$$  

(3.24)
Assuming that the eigenvalues are not degenerate \( E_n \neq E_m \forall n \neq m \) this implies

\[
|\phi^P^T_n\rangle = |\phi_n\rangle e^{i\varphi^P^T_n}.
\] (3.25)

Thus the application of the \( \mathcal{PT} \) operator to an eigenstate of the Hamiltonian in the \( \mathcal{PT} \)-symmetric regime is equivalent to a \( U(1) \) phase transformation of the eigenstate. The same argument holds for the left eigenvectors \( \langle \chi_n | \) such that one finds

\[
\langle \chi^P^T_n | = \langle \chi_n | e^{-i\varphi^P^T_n},
\] (3.26)

where the concrete value of the phase follows from the norm convention in equation (3.14). If equations (3.25) and (3.26) are used to calculate \( A^P^T_n \) from equation (3.18) one obtains a second relation of \( A_n \) and \( A^P^T_n \),

\[
A^P^T_n = i \langle \chi^P^T_n | d |\phi^P^T_n\rangle
= i \langle \chi_n | e^{-i\varphi^P^T_n} \left( i d\varphi^P^T_n |\phi_n\rangle + e^{i\varphi^P^T_n} d |\phi_n\rangle \right)
= A_n - d\varphi^P^T_n,
\] (3.27)

from which a second relation for the complex Berry phase can be calculated by integrating the Berry connection over a loop \( C \) in parameter space,

\[
\gamma^P^T_n = \oint_C A^P^T = \oint_C \left( A_n - d\varphi^P^T_n \right) = \oint_C A_n - \oint_C d\varphi^P^T_n
= \gamma_n + 2\pi z.
\] (3.28)

In the last step of equation (3.28) the integral with respect to \( d\varphi^P^T_n \) was calculated using the fact that the basis states have to be single-valued in parameter space such that one can find an integer \( z \in \mathbb{Z} \) for which the relation

\[
\oint_C d\varphi^P^T_n = -2\pi z
\] (3.29)

holds. Finally, the combination of equations (3.23) and (3.28) induce the quantisation of the real part of the complex Berry phase in the \( \mathcal{PT} \)-unbroken regime,

\[
\gamma^{(3.23)}_n = -\gamma^{P^T*}_{P^T} (3.28) = - \left( \gamma_n + 2\pi z \right)^* - \Re (\gamma_n) + i \Im (\gamma_n) = - \Re (\gamma_n + 2\pi z) + i \Im (\gamma_n)
\] (3.30)

\[
\Re (\gamma_n) = \pi z
\]

with \( z \in \mathbb{Z} \). A strict quantisation of the real part of the complex Berry phase is still present and the \( \mathcal{PT} \) symmetry protects the topological phases characterised by the real part of the complex Berry phase in such systems.

This also holds for the Zak phase, which is the Berry phase of Bloch bands in one-dimensional lattice systems. The real part of the Zak phase can be used as a topological invariant which topologically classifies the Bloch bands of one-dimensional \( \mathcal{PT} \)-symmetric lattices in the \( \mathcal{PT} \)-unbroken regime of the system (in analogy to the topological band theory of Hermitian systems).
3.2. The complex Berry phase

3.2.2. Note about the global Berry phase

Different approaches to define topological invariants for non-Hermitian systems can be found in literature. For example Liang et al. "propose[d] the global Berry phase \( Q \) of all states to identify the topological invariance" of non-Hermitian systems [18], which is defined as

\[
Q = \frac{1}{2\pi} \oint C \dim H \sum_{n=1}^{\dim H} A_n .
\] (3.31)

In the view of the author this approach is misleading and not able to characterise topological phases the way it is claimed in [18]. In the following an argument is given, which elucidates how one comes to this conclusion.

Liang et al. proved that the global Berry Phase \( Q \) is invariant modulo 1, but conclude that \( Q \) is invariant modulo \( 2\pi \). To do so, they investigated the behaviour of \( Q \) under a gauge transformation of the left and right hand eigenstates of the Hamiltonian,

\[
\langle \chi'_n | = \langle \chi_n | e^{-i\varphi_n} , \quad |\phi'_n \rangle = |\phi_n \rangle e^{i\varphi_n} ,
\] (3.32)

which induce \( \gamma'_n = \gamma_n + 2\pi \eta_n \) with arbitrary integers \( \eta_n \) analogously to the argumentation in the previous section (cf. equations (3.27) and (3.28)). Therefore, the global Berry phase transforms as

\[
Q' = \frac{1}{2\pi} \oint C \dim H \sum_{n=1}^{\dim H} A'_n = \frac{1}{2\pi} \sum_{n=1}^{\dim H} \gamma'_n
\] (3.33)

\[
= Q + \sum_{n=1}^{\dim H} \eta_n = Q + m
\]

with \( \sum \eta_n = m \in \mathbb{Z} \), and therefore

\[
Q' = Q \mod 1 .
\] (3.34)

The only values the real part of \( Q \) may take in the \( \mathcal{PT} \)-unbroken parameter regime are 0 or 1/2 modulo 1, because \( \text{Re} (\gamma_n) = \pi z \) with \( z \in \mathbb{Z} \) (see equation (3.30)). In the further course of [18] they investigated different systems and allege to identify two "topologically distinct" phases in each of them, one with \( Q = 0 \) and one with \( Q = 1 \) (so they say). Further, they claimed that between these phases "a topological phase transition occurs" and that "\( Q \) as a topological index describes the topological invariance of a system." Because of equation (3.34) the cases \( Q = 1 \) and \( Q = 0 \) are identical and invariant modulo one. Hence, even if the systems investigated in [18] possess topological distinct phases they cannot be classified by the global berry phase defined by equation (3.31). Thus, in the opinion of the author there is no reason for the global Berry phase to be able to characterise topological phases the way it is proposed in [18].
3. Biorthogonal quantum mechanics

3.2.3. The complex Berry phase in discrete parameter space

In analogy to the discrete and Hermitian case discussed in section 2.1.1 the complex Berry phase can be written as

$$\gamma_n = i \ln \left( \prod_{j=1}^{M} \langle \chi_{n,j} | \phi_{n,j+1} \rangle \right),$$  \hspace{1cm} (3.35)

where again the eigenstates \(\{\langle \chi_{n,j} |, | \phi_{n,j} \rangle\}\) correspond to the point \(\alpha_j\) of the discretised loop \(C = (\alpha_1, ..., \alpha_j, ..., \alpha_M = \alpha_1)\) and periodic boundary conditions \(M + 1 \equiv 1\). The phase factor

$$e^{i\gamma_n} = \prod_{j=1}^{M} \langle \chi_{n,j} | \phi_{n,j+1} \rangle = \prod_{j=0}^{M-1} e^{i\gamma_{n,j+1}}$$  \hspace{1cm} (3.36)

picked up by a pair of biorthogonal eigenstates which are transported through the parameter space has the same interpretation as in the Hermitian case. The states pick up a phase for every step along the loop \(C\). But now one needs to consider the biorthogonal projections of the neighbouring basis states. This is illustrated in figure 3.1. The definition of the complex Berry phase in equation (3.35) is again immanently \(U(1)\) gauge invariant if one defines a gauge transformation as a transformation of a state of the Hilbert space and a simultaneous transformation of its biorthogonal partner in the dual Hilbert space,

$$|\phi_{n,j} \rangle \longrightarrow e^{i\varphi_{n,j}} |\phi_{n,j} \rangle, \hspace{1cm} \langle \chi_{n,j} | \longrightarrow e^{-i\varphi_{n,j}} \langle \chi_{n,j} |.$$  \hspace{1cm} (3.37)

In the example of the complex Zak phase (the Berry phase with the first Brillouin zone acting as loop in parameter space) the requirements for the equivalence of the two different definitions of the complex Berry phase (cf. equations (3.17) and (3.35)) can be shown. The following argument works analogously for Hermitian systems where one substitutes the left hand eigenvector by the Hermitian adjoint of the right hand eigenstate, \(\langle \chi_n | = (|\phi_n \rangle^*)^T\). In the following \(\{\langle \chi_n(k_j) |, | \phi_n(k_j) \rangle\}\) is a biorthogonal basis of the Bloch Hamiltonian \(H(k_j)\) and \(BZ = (k_1, ..., k_j, ..., k_M = k_1)\) is the discretised Brillouin zone acting as loop in parameter space. The continuous circuit integral occurring in the definition of the Zak phase and the derivative with respect to \(k\) (cf. equation (3.17)) can be discretised,

$$\gamma_n = i \oint_{BZ} \langle \chi_n(k) | \partial_k | \phi_n(k) \rangle \, dk$$

$$= i \lim_{M \to \infty} \lim_{\Delta k \to 0} \frac{2\pi}{M} \sum_{j=1}^{M} \frac{1}{\Delta k} \left( \langle \chi_{n,j} | \phi_{n,j+1} \rangle - \langle \chi_{n,j} | \phi_{n,j} \rangle \right)_{=1 (norm)} \hspace{1cm} (3.38)$$

$$= i \lim_{M \to \infty} \sum_{j=1}^{M} \left( \langle \chi_{n,j} | \phi_{n,j+1} \rangle - 1 \right),$$
3.2. The complex Berry phase

Shapes:

|φ3⟩
⟨χ3|
|φ2⟩
⟨χ2|
|φ1⟩
⟨χ1|

Figure 3.1.: Schematic loop in a discrete parameter space. Here the index \( n \) was dropped for matters of clarity. A pair of biorthogonal states picks up a phase for every step in the discretised parameter space.

where \( |φ_{n,m+1}⟩ = |φ_n(k_m + Δk)⟩ \) and \( M + 1 ≡ 1 \) because of the periodic boundary conditions of the Brillouin zone. In the first step of equation (3.38) the relations

\[
\int_a^b f(x)dx = \lim_{M→∞} \frac{b-a}{M} \sum_{n=1}^M f(x_n), \quad (3.39)
\]

\[
∂_xf(x) = \lim_{h→0} \frac{f(x+h) - f(x)}{h}, \quad (3.40)
\]

were used to discretise the Zak phase. The discrete definition of the Zak phase (cf. equation (3.35)) can be brought to the same form. Therefore one assumes the deviation of the biorthogonal scalar product from 1 to be small, such that a first-order approximation of the logarithm is reasonable,

\[
γ_n = i \ln \left( \prod_{j=0}^{M-1} ⟨χ_{n,j}|φ_{n,j+1}⟩ \right)
\]

\[
= i \sum_{j=1}^M \ln \left( ⟨χ_{n,j}|φ_{n,j+1}⟩ - 1 + 1 \right)_{x_{n,j}}
\]

\[
= i \sum_{j=1}^M \sum_{p=1}^{∞} \frac{(-1)^{p+1} x^p}{p}
\]

\[
\approx \left( x_{n,j} \right)_{p=1}^M
\]

\[
= i \sum_{j=1}^M \left( ⟨χ_{n,j}|φ_{n,j+1}⟩ - 1 \right), \quad (3.41)
\]

where the series expansion \( \ln(x + 1) = \sum_{p=1}^{∞} \frac{(-1)^{p+1} x^p}{p} \) was used in the second step. As long as \( x_{n,j} \) is small this result of equation (3.41) is equal to the discretisation of the exact formula of the Zak phase in equation (3.38). For small discretisation steps in the Brillouin zone the modulus of the scalar product of neighbouring biorthogonal basis
states is close to 1 and therefore $|x_{n,j}| \approx 0$, and the approximation is justified. Later on in this thesis complex Zak phases of non-Hermitian Bloch Hamiltonians are investigated, where this approximation is no longer justified as exceptional points may occur in the $\mathcal{PT}$-broken regime, for which surrounding the approximation is no longer valid because of the self-orthogonality of the biorthogonal basis, which causes $|x_{n,j}| \approx 1$. Therefore another method for the calculation of complex berry phases is needed. The construction of such a method is the topic of the next chapter.
4. Numerical method

In this Chapter a numerical method [46] is presented, which is required in all cases with nontrivial complex potentials preventing a completely analytical evaluation of the eigenvectors of the Hamiltonian. This method is used to compute complex Zak phases of different lattice systems in the remaining part of this thesis. Thereby an appropriate smoothed gauge of the biorthogonal basis of non-Hermitian Hamiltonians is constructed along a discretised loop $\mathcal{C}$ in parameter space such that integrals of the form

$$\oint_{\mathcal{C}} \langle \chi_n | \nabla_{\alpha} | \phi_n \rangle \cdot d\alpha$$

become solvable numerically.

The algorithm is applicable to non-Hermitian as well as Hermitian systems (see chapter 5) and to dissipative systems described in the framework of Lindblad master equations in third quantization (see chapter 6) allowing for the numerical calculation of Berry phases without a special treatment of exceptional points occurring in the parameter space. The loop in parameter space will be the first Brillouin zone, where the other parameter values are fixed throughout this work, however the algorithm in principle allows for the investigation of all other loops.

Numerical gauge smoothing

In the following a numerical method to construct a smoothed gauge for the left and right hand eigenvectors $\langle \chi_n |$ and $| \phi_n \rangle$ of non-Hermitian Hamiltonians is presented. This allows for the computation of complex Berry phases on discretised loops $\mathcal{C} = (\alpha_1, ..., \alpha_j, ..., \alpha_M = \alpha_1)$ in parameter space.

At every point $\alpha_j$ of the discretised loop $\mathcal{C}$ the left and right hand versions of the time-independent Schrödinger equation,

$$\langle \chi_n(\alpha_j) | H(\alpha_j) | \chi_n(\alpha_j) \rangle = E_n(\alpha_j) \langle \chi_n(\alpha_j) |$$

$$H(\alpha_j) | \phi_n(\alpha_j) \rangle = E_n(\alpha_j) | \phi_n(\alpha_j) \rangle,$$

define a set of unnormalised natural left and right basis states $\{ \langle \chi_n(\alpha_j) |, | \phi_n(\alpha_j) \rangle \}$ and provide the eigenvalues $E_n$. All these eigenvectors are calculated numerically and possess an independent phase, which is a priori neither equal for left and right hand eigenstates nor smooth or correlated between different points in parameter space. At this stage
4. Numerical method

Shapes:

\[ |\phi\rangle \langle \chi| \alpha_{j-1} \quad \cdots \quad |\phi\rangle \langle \chi| \alpha_j \quad \cdots \quad |\phi\rangle \langle \chi| \alpha_{j+1} \quad \cdots \]

\[ e^{i\eta_{j-1,j}} \quad e^{i\eta_{j,j+1}} \]

Figure 4.1.: Schematic illustration of unnormalised states in a discrete parameter space exemplifying the different phases occurring in the numerically calculated eigenbasis of the Hamiltonian. The phase \( \xi \) occurs locally between the states at each point \( \alpha_j \), whereas the phase \( \eta_{j,j+1} \) appears between the states of neighbouring points in parameter space.

the phases of the two basis states at every point of \( C \) disturb two phase relations, one between each pair of the left and right hand eigenstates at a given \( \alpha_j \) and one between the eigenstates of neighbouring points \( \alpha_j \) and \( \alpha_{j+1} \) belonging to the same branch of eigenvalues. This situation is depicted in figure 4.1. The biorthogonal normalisation condition [56],

\[
\langle \chi_n(\alpha_j) \rangle \rightarrow \frac{\langle \chi_n(\alpha_j) \rangle}{\sqrt{\langle \chi_n(\alpha_j) | \phi_n(\alpha_j) \rangle}}, \quad (4.3a)
\]

\[
|\phi_n(\alpha_j)\rangle \rightarrow \frac{|\phi_n(\alpha_j)\rangle}{\sqrt{\langle \chi_n(\alpha_j) | \phi_n(\alpha_j) \rangle}}, \quad (4.3b)
\]

fixes the phase relation between the left and right eigenstates (cf. the phases \( \xi \) in figure 4.1) locally by choosing one arbitrary global phase for each point \( \alpha_j \). After the sole application of the substitution given by equations (4.3a) and (4.3b) the pursued smoothed gauge would still be distorted by the phases which occur between the states of neighbouring points in parameter space (cf. the phases \( \eta \) in figure 4.1). For the evaluation of local properties this would be sufficient, however the calculation of the Berry phase demands for the evaluation of a circuit integral in parameter space involving different points. Hence a phase relation between consecutive steps connecting neighbouring points in parameter space (cf. the phases \( \eta \) in figure 4.1) that does not distort the result of a numerical integration of equation (3.17) has to be established.

Hence an arbitrary global phase is chosen for the basis states of one specific point and transfers this choice onto the states at all other points of the discretised loop \( C \). This transfer is split into a two-stage procedure, for which the first point of the loop \( \alpha_1 \) is a convenient starting point. To this end, one applies the normalisation condition from equations (4.3a) and (4.3b) simultaneously on all basis states at the point \( \alpha_1 \) and thereby chooses one arbitrary global phase for the states \( \langle \chi_n(\alpha_1) \rangle \) and \( |\phi_n(\alpha_1)\rangle \). This phase is transferred iteratively onto the neighbouring states \( \langle \chi_n(\alpha_j) \rangle \) and \( |\phi_n(\alpha_j)\rangle \) by
applying the substitution rule
\[ \langle \chi_n(\alpha_j) \rangle \to \langle \chi_n(\alpha_j) \rangle e^{-i \arg(\langle \chi_n(\alpha_j) | \phi_n(\alpha_{j-1}) \rangle)} , \]  
and
\[ |\phi_n(\alpha_j)\rangle \to |\phi_n(\alpha_j)\rangle e^{-i \arg(\langle \chi_n(\alpha_{j-1}) | \phi_n(\alpha_j) \rangle)} \]  
and the normalisation condition given by equations (4.3a) and (4.3b) for \( j \in \{2, ..., M\} \).

As a result of the application of equations (4.4a) and (4.4b) a relation between the basis states of neighbouring points \( \alpha_j \) and \( \alpha_{j+1} \) is constructed by ensuring
\[ \text{Im}(\langle \chi_n(\alpha_j) | \phi_n(\alpha_{j-1}) \rangle) = 0 , \]  
(4.5a)
\[ \text{Im}(\langle \chi_n(\alpha_{j-1}) | \phi_n(\alpha_j) \rangle) = 0 , \]  
(4.5b)
which is a valid condition in the continuous limit \( \alpha_j \to \alpha_{j+1} \). The application of the normalisation conditions (4.3a) and (4.3b) force the basis states to fulfil
\[ \langle \chi_m(\alpha_j) | \phi_n(\alpha_j) \rangle = \delta_{mn} \]  
(4.6)
for \( j \in \{1, ..., M\} \) and for all \( n \) and \( m \).

At this stage of the process the gauge of the biorthogonal basis is smooth along the loop \( C \) between the first and last point, but the biorthogonal basis is not yet single-valued in the parameter space, which is essential for the calculation of a Barry phase [12]. In particular, the vectors at the first and the last point of the loop have to be identical, which is not necessarily the case at this stage. The equality of these vectors can be ensured by compensating the phase difference occurring between the states \( \langle \chi_n(\alpha_1) \rangle \) and \( \langle \chi_n(\alpha_M) \rangle \), respectively, as well as \( |\phi_n(\alpha_1)\rangle \) and \( |\phi_n(\alpha_M)\rangle \). This statement remains true for the components of these vectors.

One calculates the phase difference between the first non-vanishing component \( p \) of the left basis states \( \langle \chi_n(\alpha_1) \rangle \) and \( \langle \chi_n(\alpha_M) \rangle \),
\[ \Delta \varphi_n = \varphi_{n,M} - \varphi_{n,1} + 2\pi X_n , \]  
(4.7)
where \( \varphi_{n,j} = \arg(\langle \chi_n(\alpha_j) | p \rangle) \) is the argument of component \( p \) of the left eigenvector at the point \( \alpha_j \) in parameter space and \( X \) denotes the sum of directed crossings of the phase \( \varphi_{n,j} \) over the borders of the standard interval \([−\pi, \pi)\). Starting with \( X = 0 \) one increases \( X \) by one for every jump of \( \varphi_{n,j} \) from \(-\pi \) to \( \pi \) and subtracts 1 for a jump in the opposite direction. To ensure the equality and simultaneously maintain the smoothness of the gauge along the loop connecting \( \alpha_1 \) and \( \alpha_M \) one multiplies the states at \( \alpha_j \) by a phase factor according to
\[ \langle \chi_n(\alpha_j) \rangle \to \langle \chi_n(\alpha_j) \rangle e^{-i f \Delta \varphi_n ((j-1)/(M-1))} , \]  
(4.8a)
\[ |\phi_n(\alpha_j)\rangle \to |\phi_n(\alpha_j)\rangle e^{i f \Delta \varphi_n ((j-1)/(M-1))} \]  
(4.8b)
4. Numerical method

for \( j \in \{1, \ldots, M\} \), where \( f_{\Delta \varphi_n}(x) \) is any “smooth” real valued and continuous function

\[
f_{\Delta \varphi_n} : [0, 1] \to \mathbb{R}
\]

fulfilling:

\[
0 \mapsto f_{\Delta \varphi_n}(0) = 0
\]

\[
1 \mapsto f_{\Delta \varphi_n}(1) = \Delta \varphi_n \pm 2\pi z
\]

with \( z \in \mathbb{Z} \). The explicit form of the gauge function \( f_{\Delta \varphi_n}(x) \) is not critical since it only corrects the total phase change of the states along the entire loop, which is a result of the first stage of the process. However, a linear gauge function, which is the simplest function fulfilling the conditions in equation (4.9b), turns out to be a good choice.

Figure 4.2 shows a simplified flow chart of the algorithm. As a result of the first step of the gauge smoothing procedure (cf. red shaded area in figure 4.2) the arbitrary global phases have been removed. Only one arbitrary phase is left, which has no influence, since it is identical for all right eigenvectors and its complex conjugate for all left eigenvectors. The second step (cf. green shaded area in figure 4.2) finally smoothes the gauge by ensuring the uniqueness of the basis in parameter space by compensating the phase difference between the first and last point of the loop, which are identical. Note that the algorithm can theoretically handle Hamiltonians of arbitrary dimensions, but as all eigenvectors have to be saved until the complex Berry Phase is computed the dimension of the Hamiltonian and the size of the discretisation steps of the loop are restricted by the available memory and the finiteness of the computation time.
Figure 4.2: Simplified flow chart of the algorithm used to calculate complex Berry phases. The input of the algorithm is a Hamiltonian depending on parameters $\alpha \in \mathbb{P}$ and a loop $C \subset \mathbb{P}$ in parameter space $\mathbb{P}$. The background colours mark the two parts of the gauge smoothing procedure. The orange area illustrates the first part, whereas the green area marks the second step, in which the basis is made unique within the discretised curve $C$. The algorithm is completed by a numerical integration of equation (3.17).
5. **$\mathcal{PT}$-symmetric lattice systems**

In this chapter open lattice systems are studied in an effective description using $\mathcal{PT}$-symmetric Hamiltonians. All lattices possess a translational symmetry allowing for the construction of a Fourier representation of the Hamiltonian, and thus a Bloch Hamiltonian can be constructed. This non-Hermitian Bloch Hamiltonian allows for a non-Hermitian, $\mathcal{PT}$-symmetric generalization of the Hamiltonian band theory for open lattice systems in the scope of the effective description. The algorithm presented in chapter 4 is applied on this Bloch Hamiltonian to calculate the Zak phases of each energy band to topologically classify the band structure in the $\mathcal{PT}$-unbroken regime. In this process the loop in parameter space is given by the first Brillouin $\mathcal{BZ}$ zone where $k \in \mathcal{BZ} \leftrightarrow k \in [-\pi/a, \pi/a)$. The gauge function (cf. equation (4.9a)) is chosen to be

$$f_{\Delta \varphi_n}(x) = \Delta \varphi_n x - 2\pi$$

with

$$x = \frac{k + \pi/a}{2\pi/a},$$

which is the most simple function fulfilling the conditions (4.9b). From now on the scaling parameter $a$ is set to one, $a = 1$.

5.1. **SSH model**

In the following different $\mathcal{PT}$-symmetric extensions of the SSH model are investigated. The Hamiltonian with fermionic creation and annihilation operators $c$ and $c^\dagger$,

$$H_{\text{SSH}} = \frac{N}{2} \sum_{n=1}^{N/2-1} t_- \left( c_{A_n}^\dagger c_{B_n} + \text{h.c.} \right) + \sum_{n=1}^{N/2-1} t_+ \left( c_{B_n}^\dagger c_{A_{n+1}} + \text{h.c.} \right)$$

(5.2)

describes the SSH model without a complex on-site potential, which is illustratively discussed in section 2.2.1. Throughout this thesis the tunnelling amplitudes $t_\pm = t \left( 1 \pm \Delta \cos(\theta) \right)$ are parametrised by the tunnelling strength $t$, the dimerisation strength $\Delta$ and the dimerisation parameter $\theta$. Consequently, it holds $t_+ > t_-$ for $\theta \in [0, \pi/2)$, $t_+ < t_-$ for $\theta \in (\pi/2, \pi]$, and $t_+ = t_-$ for $\theta = \pi/2$. All considerations are restricted to the interval $\theta \in [0, \pi]$. In the following different $\mathcal{PT}$-symmetric on-site potentials with a parameter of gain and loss $\Gamma$ are applied to the SSH model, and their Zak phase as well as the energy bands are calculated from their Bloch Hamiltonian. To do so, the
5. \( \mathcal{PT} \)-symmetric lattice systems

parameters \( t, \theta, \Delta \) and \( \Gamma \) are held constant while \( k \) is varied from \(-\pi\) to \( \pi\) to close a loop in the parameter space. Throughout this work potentials with positive values of \( \Gamma \) are investigated. For \( \Gamma < 0 \) the particle sinks and sources are interchanged leading to a spatially reflected system with the same general properties as the system with \( \Gamma > 0 \).

The complex Zak phase is used to investigate the topology of the bulk, by classifying the topology of the band structure using its real part. To substantiate the detection of a possible topologically nontrivial phase, which is indicated by a complex Zak phase with a real part of \( \pi \), the ground states of the many-body Hamiltonian are investigated. The ground state is expected to show topologically nontrivial properties if the sum over the Zak phases of all bands with negative energies is nontrivial (equal to \( \pi \) mod \( 2\pi \)). To investigate the ground states the method of exact diagonalisation is used. This is done by setting up the many-body Hamiltonian in the Fock basis and using the ARPACK library [59] to calculate its ground states and the corresponding complex energies (the states with a minimal real part of the complex energy). As \( \mathcal{PT} \) symmetry is used as an effective description of open quantum systems, observables are evaluated similarly to the procedure in Hermitian quantum mechanics by using the right hand eigenstates of the Hamiltonian. The ground states are relevant because some of the results which are investigated in this section are compared to the dynamical steady states obtained from an investigation of analogous systems in the Lindblad formalism (see chapter 6). Thus states with higher energies would violate the assumption of minimal coupling of system and bath coordinates, which is essential in the derivation of the Lindblad master equation.

Typically one can find a number of different ground states in \( \mathcal{PT} \)-symmetric many-body systems, which are degenerate according to the real part of their complex energy eigenvalue. Besides the \( \mathcal{PT} \)-unbroken ground state (with a real energy eigenvalue) the \( \mathcal{PT} \)-broken ground state with the maximal imaginary part of the complex energy eigenvalue is of interest. In the following this state is called maximal \( \mathcal{PT} \)-broken ground state. This state becomes dominant in a unitary-like time evolution in the effective description of open systems used in this chapter.

5.1.1. Alternating gain and loss

The on-site potential describing alternating gain and loss in an one-dimensional lattice is given by

\[
U_{\text{alt}} = \frac{\Gamma}{2} \sum_{n=1}^{N/2} \left(c_{A_n}^\dagger c_{A_n} - c_{B_n}^\dagger c_{B_n}\right), \tag{5.3}
\]

where \( \Gamma \) denotes the parameter of gain and loss. Figure 5.1 shows an illustrative sketch of the SSH model subject to this complex potential. The \( \mathcal{PT} \)-symmetric Hamiltonian describing this system is given by (cf. equation (5.2))

\[
H = H_{\text{SSH}} + U_{\text{alt}} \tag{5.4}
\]
5.1. SSH model

Figure 5.1.: Schematic sketch of the SSH model with tunnelling amplitudes \( t_- \) and \( t_+ \) subject to an alternating imaginary potential. The minus signs mark sites with negative imaginary potential corresponding to sinks of the probability density, plus signs mark sites with positive imaginary potential corresponding to sources of the probability density.

on which a Fourier transformation can be applied following appendix A resulting in the Bloch Hamiltonian

\[
\mathcal{H} = \begin{pmatrix}
\frac{i\Gamma}{2} & t_- + t_+ e^{ik} \\
 t_- + t_+ e^{-ik} & -\frac{i\Gamma}{2}
\end{pmatrix}.
\]  

(5.5)

This matrix can be decomposed into the Pauli matrices

\[
\mathcal{H}(k) = (t_- + t_+ \cos(k)) \sigma_1 - t_+ \sin(k) \sigma_2 - i\Gamma/2 \sigma_3
\]

\[
= \mathbf{n}(k) \cdot \boldsymbol{\sigma}
\]

(5.6)

with a coefficient vector \( \mathbf{n}(k) \) and the Pauli vector \( \boldsymbol{\sigma} \). From this form the energy eigenvalues can be obtained explicitly,

\[
E_{\pm}(k) = \pm |\mathbf{n}(k)|.
\]  

(5.7)

In the limit \( \Gamma \to 0 \) the Hamiltonian from equation (5.5) reproduces the Hermitian SSH model, which possesses time-reversal, reflection, particle-hole, and a chiral symmetry (represented by \( \sigma_3 \)). The introduction of a \( \mathcal{PT} \)-symmetric non-Hermitian on-site potential \( \Gamma \) breaks these symmetries. The non-Hermitian Bloch Hamiltonian is invariant under the combined action of the parity operator \( \mathcal{P} \) and the time inversion operator \( \mathcal{T} \). Further the particle-hole symmetry is broken because the sources (sinks) of an electron correspond to sinks (sources) of holes. The non-Hermitian system is therefore invariant under the action of the combination of the parity and the charge conjugation operator. Further it has no chiral symmetry \( \Lambda = a_0 \sigma_0 + a \cdot \boldsymbol{\sigma} \) because a chiral symmetry would fulfil

\[
\{ \Lambda, \mathcal{H} \} = \sum_{i=0}^{3} \sum_{j=1}^{3} a_i n_j \{ \sigma_i, \sigma_j \}
\]

(5.8)

\[
= 2(a_1 n_1 + a_2 n_2 + a_3 n_3) \sigma_0 + 2a_0 \sum_{j=1}^{3} n_j \sigma_j
\]

\[
\equiv 0
\]
with a coefficient vector \( \mathbf{a} \) which is independent of the value of \( k \), the \( 2 \times 2 \) identity matrix \( \sigma_0 \), and the anti-commutation relations \( \{ \sigma_i, \sigma_j \} = 2 \delta_{ij} \sigma_0 \) of the Pauli matrices. Therefore, one finds \( a_0 = 0 \), and thus

\[
a_1 n(k)_1 + a_2 n(k)_2 + a_3 n_3 \equiv 0 ,
\]

which cannot be satisfied for a constant vector \( \mathbf{a} \) because the vector \( \mathbf{n}(k) \) rotates on a cylindrical surface as \( k \) runs through the Brillouin zone. Hence the non-Hermitian Bloch Hamiltonian in equation (5.5) does not possess a chiral symmetry. However, this does not mean that there is no quantised real part of the complex Zak phase since its quantisation is ensured by the argument of Hatsugai [58] in the \( \mathcal{PT} \)-unbroken parameter regime as shown in section 3.2.1. Thus, the quantisation of the Berry phase in the \( \mathcal{PT} \)-unbroken parameter regime is not the result of a chiral symmetry but rather the topological phases are protected by the \( \mathcal{PT} \) symmetry.

In the following, the \( \mathcal{PT} \)-symmetric SSH model with alternating gain and loss is used to test the numerical method presented in chapter 4 as the system is analytically accessible. The numerical results of the complex Zak phases are computed using the algorithm introduced in chapter 4. As mentioned above, the coordinates \( t, \Delta, \theta \) and \( \Gamma \) of the parameter space \( \mathbb{P} \) are held constant while \( k \) runs once through the Brillouin zone \( \mathbb{BZ} \subset \mathbb{P} \) to close a loop, on which a gauge smoothed biorthogonal basis of eigenstates is constructed, which is used in the numerical integration of equation (3.17). To verify these results they are compared to the analytical ones derived in [18],

\[
\gamma_{0/1} = \pi \Theta(q - 1) \pm \frac{\eta}{2} \sqrt{\nu} \left( K(\nu) + \frac{q - 1}{q + 1} \Pi(\mu, \nu) \right) , \tag{5.10}
\]

where \( q = t_+/t_- \) is the ratio of the tunnelling amplitudes, \( \eta = \Gamma/(2t_-) \), \( \nu = 4q/((q + 1)^2 - \eta^2) \), and \( \mu = 4q/(q + 1)^2 \). \( K(\nu) \) and \( \Pi(\mu, \nu) \) are elliptic integrals of first and third kind,

\[
K(\nu) = \int_{0}^{\pi/2} \frac{dk}{\sqrt{1 - \nu \sin^2(k)}} , \tag{5.11}
\]

\[
\Pi(\mu, \nu) = \int_{0}^{\pi/2} \frac{dk}{1 - \mu \sin^2(k) \sqrt{1 - \nu \sin^2(k)}} . \tag{5.12}
\]

Figures 5.2 (a) and (b) contain the analytical results and that obtained by a numerical integration of equation (3.17). They perfectly reproduce each other for all values of \( \theta \). The grey shaded area marks the \( \mathcal{PT} \)-broken parameter regime. The real part of the complex Zak phase is quantised in the \( \mathcal{PT} \)-unbroken regime and it can be used to characterise the topological phase of the system.
5.1. SSH model

Figure 5.2.: In (a) and (b) the analytical (real and imaginary part are represented by a solid black line coinciding with the numerical results) and numerical results obtained by a numerical integration of equation (3.17) (solid red line and open blue circles) of the complex Zak phase of the SSH model with alternating gain and loss are shown in dependence of the dimerisation parameter \( \theta \). The other system parameters are \( t = 1, \Delta = 1/2 \) and \( \Gamma = 1 \) (all values in a.u.). The complex Zak phases can be calculated alternatively by using the gauge smoothed biorthogonal basis of eigenstates to solve the coupled differential equation system (3.16) with initial conditions \( c_0(0) = 1, c_1(0) = 0 \) in (a) and \( c_0(0) = 0, c_1(0) = 1 \) in (b). The results of this computation are represented by green crosses (real part) and orange stars (imaginary part). All results match each other perfectly. This alternative computation is just of demonstrative purpose. In the following the numerical results are always obtained by a numerical integration of equation (3.17). The grey shaded area marks the \( \mathcal{PT} \)-broken parameter regime, where the eigenvalues of the Bloch Hamiltonian are complex somewhere in the Brillouin zone. The real part of the complex Zak phase is quantised in the \( \mathcal{PT} \)-unbroken regime where the eigenvalues of the Bloch Hamiltonian are entirely real independently of the value of \( k \). On the right hand side, the first component of the left hand eigenvector \( \langle \chi_0(\alpha_j) | 1 \rangle \) corresponding to \( \gamma_0 \) (cf. (a)) is depicted in dependence of the wave number \( k \) with \( t = 1, \Delta = 1/2, \Gamma = 1 \) and \( \theta \approx 0.3 \pi \). (c) Before the steps described in equations (4.4a) and (4.4b) one can identify two different phase branches (blue lines) and a constant modulus (filled red dots). (d) After the steps characterised by equations (4.3a) and (4.3b) (here \( \Delta \tilde{\varphi}_1 = \varphi_{M,1} - \varphi_{1,1} \) and \( X = -1 \) c.f. eq. (4.7)) the phase is smooth within the Brillouin zone but discontinuous at its boundaries, and the modulus varies with \( k \). (e) After the gauge smoothing process the phase difference \( \Delta \tilde{\varphi}_1 \) is compensated and the phase is continuous and smooth in the whole Brillouin zone.
Figure 5.3.: Complex Zak phases of the SSH model with alternating imaginary potential in dependence of the dimerisation parameter $\theta$ and the parameter of gain and loss $\Gamma$. The system parameters are $t = 1$ and $\Delta = 0.5$. The topologically (non)trivial phase is represented by the grey (green, lighter grey area in a black and white printout) area. The complex Zak phase $\gamma_0$ ($\gamma_1$) corresponds to the eigenvalue branch being always negative (positive) for $k = 0$ (cf. figure 5.4). The hatched area marks the $\mathcal{PT}$-broken parameter regime for which the energy eigenvalues corresponding to the eigenstates used to calculate the Zak phase have a nonvanishing imaginary part somewhere in the first Brillouin zone.

Here and in the following the $\mathcal{PT}$ symmetry of the system is said to be broken respectively unbroken if the eigenvalues of the Bloch Hamiltonian are complex for one value of $k$ respectively entirely real-valued for all values of $k$. In contrast, the many-body states of a finite version of the lattice model, which will be investigated later on in this section, may be $\mathcal{PT}$-broken in the parameter regime which is here called $\mathcal{PT}$-unbroken and vice versa.

In the $\mathcal{PT}$-unbroken regime, the results can be confirmed by an alternative analysis. The gauge smoothed biorthogonal basis of eigenstates can be used to solve the coupled differential equation system (3.16) with initial conditions $c_0(0) = 1, c_1(0) = 0$ to obtain $\gamma_0$ and initial conditions $c_0(0) = 0, c_1(0) = 1$ for $\gamma_1$. For example, by using a Runge–Kutta method. The purpose of this alternative computation is merely to demonstrate that the approximations used in (3.2) to obtain equation (3.17) are reasonable. In the upcoming parts of this thesis, the numerical results of the complex Zak phase are always obtained by a numerical integration of equation (3.17).

The numerical gauge smoothing process is exemplified in the following. For this purpose, the first component of a left eigenvector is depicted on the right hand side of figure 5.2 for different stages of the gauge smoothing procedure. The unnormalised component $\langle \chi_0(\alpha_j) | 1$ before the gauge smoothing process is shown in Figure 5.2 (c). One can see two different phase branches as a result of the numerical diagonalisation and a constant
5.1. SSH model

modulus. After the first step of the gauge smoothing process described in chapter 4 the modulus varies with the wave number \( k \) and there is only one phase branch left, but the basis is not yet single-valued as there is still a phase difference at the boundaries of the Brillouin zone as shown in Figure 5.2 (d). In this example the factor \( X = -1 \) (cf. equation (4.7)) has to be used as \( \varphi_{0,j} \) jumps from \( -\pi \) to \( \pi \). After the second step of the algorithm the component \( \langle \chi_0(\alpha_j) | 0 \rangle \) of the gauge smoothed left eigenvector is unambiguous in the whole Brillouin zone (especially at the Brillouin zone boundaries) as shown in figure 5.2 (e).

If one varies the parameter of gain and loss \( \Gamma \) and the dimerisation parameter \( \theta \), and calculates the Zak phase \( \gamma \) for a fixed tunnelling strength \( t \) and dimerisation strength \( \Delta \), one obtains the phase diagram shown in figure 5.3. A topologically nontrivial phase is indicated by \( \text{Re}(\gamma) = \pi \) (green coloured areas, lighter grey colour in a black and white printout), and \( \text{Re}(\gamma) = 0 \) indicates a topologically trivial phase. In the \( \mathcal{PT} \)-unbroken phase the real part of the complex Zak phase is quantised and takes the same values as the SSH model without a complex potential, which is reproduced for \( \Gamma \to 0 \). At the \( \mathcal{PT} \) phase transitions the imaginary part of the complex Zak phase diverges (cf. also figure 5.2 (a) and (b)). One can identify two topologically distinct phases. One topologically nontrivial phase with \( \text{Re}(\gamma) = \pi \) for \( \theta < \pi/2 \) and a topologically trivial phase with \( \text{Im}(\gamma) = 0 \) for \( \theta > \pi/2 \).

The band structure of the model is shown in figure 5.4 for different values of \( \theta \). The complex energy bands are gapped in the \( \mathcal{PT} \)-unbroken parameter regimes, where the real part of the complex Zak phase is quantised. The band gap closes at the \( \mathcal{PT} \) phase transition at \( k = \pm \pi \). The degenerate points are exceptional points which move towards the centre of the Brillouin zone when one varies the value of \( \theta \) towards the centre of the
5. \(\mathcal{PT}\)-symmetric lattice systems

\begin{figure}[h]
\centering
\includegraphics{figure55.png}
\caption{Ground state expectation values of the occupation number operator \(\langle n \rangle\) for the SSH model with 16 lattice sites subject to an alternating imaginary potential \(U_{\text{alt}}\) (cf. equation (5.3)) with \(t = 1, \Delta = 0.5\) and \(\Gamma = 1.4\). For \(\theta = \pi/16\) a \(\mathcal{PT}\)-unbroken ground state is shown in (a) which has the same real part of the energy as the maximal \(\mathcal{PT}\)-broken ground state shown in (b). For \(\theta = \pi\) the states are shown in (c) and (d). In (c) a \(\mathcal{PT}\)-unbroken ground state is shown and in (d) the maximal \(\mathcal{PT}\)-broken ground state. These states have again the same real part of the energy. The maximal \(\mathcal{PT}\)-broken ground states have higher occupation number operator expectation values on sites with a positive complex potential describing particle gain.}
\end{figure}

\(\mathcal{PT}\)-broken parameter regime in figure 5.3. Thus this scenario can be compared to the Hermitian case of the SSH model, but now the band gap is closed for an interval of \(\theta\) and not only for \(\theta = \pi/2\), where the phase transition occurs in the Hermitian case.

As there is only one band with \(\text{Re}(E) < 0\) in the \(\mathcal{PT}\)-unbroken parameter regime the ground state is expected to show the same topological phases as the low energy eigenstate of the Bloch Hamiltonian. Thus, the ground states of a finite version of this model are investigated in the following by using the method exact diagonalisation of the many-body Hamiltonian using the ARPACK library [59] as mentioned above. This examination of the ground states should clarify weather edge states can be found in the topologically nontrivial phase, as they indicate a nontrivial topology.

The expectation values of the occupation number operators with respect to states of a finite lattice without periodic boundary conditions are depicted in figure 5.5 for parameter values of the two \(\mathcal{PT}\)-unbroken and topologically distinct phases indicated by the Zak phases shown in figure 5.3. The exact form of the phases may change in this case because of finite size effects. For the topologically nontrivial phase, characterised by \(\text{Re}(\gamma) = \pi\), two different ground states are shown in (a) and (b). The degenerate \(\mathcal{PT}\)-unbroken ground states with a real energy are edge states. One of them is depicted in figure 5.5 (a). The other \(\mathcal{PT}\)-unbroken ground state looks like the image of the state shown in (a) reflected at an imagined line at \(\langle n \rangle = 0.5\). The maximal \(\mathcal{PT}\)-broken ground state is drawn in (b), where the influence of the complex potential reveals itself by an alternating expectation value of the occupation number operator. Sites with a positive imaginary potential are more likely to be occupied. The maximal \(\mathcal{PT}\)-broken ground state is not a topological state in the sense of Hermitian quantum mechanics because it is not degenerate, even though it has the same the real part of the complex eigenvalue.
5.1. SSH model

Figure 5.6.: Schematic sketch of the SSH model with tunnelling amplitudes $t_-$ and $t_+$ analogously to figure 5.1. In addition it allows for second-neighbour hopping with a constant amplitude $t_{2nd}$.

But a comparison with the steady states of an analogous system in the framework of Lindblad master equations (cf. section 6.3.1) will show that this state reproduces the occupation number expectation values of the dynamical steady state.

For the topologically trivial phase, characterised by $\text{Re}(\gamma) = 0$, a $\mathcal{PT}$-unbroken ground state is shown in figure 5.5 (c). Like this state, all coexisting states found in this regime exhibit no striking edge occupation. The maximal $\mathcal{PT}$-broken ground state is shown in (d). Again the dynamical steady state of an analogous system in the framework of Lindblad master equations has very similar occupation number expectation values as the maximal $\mathcal{PT}$-broken ground state. The discussion of this analogy is part of the next chapter (see section 6.3).

**Alternating gain and loss with second-neighbour hopping**

If one extends the Hamiltonian from equation (5.2) by a second-neighbour hopping term with a constant amplitude and applies an alternating complex potential $U_{\text{alt}}$ given by equation (5.3), one obtains the Hamiltonian

$$H = H_{\text{SSH}} + U_{\text{alt}} + \sum_{n=1}^{N/2} t_{2nd} \left( c_{A_n}^{\dagger} c_{A_{n+1}} + c_{B_n}^{\dagger} c_{B_{n+1}} + \text{h.c.} \right) ,$$

which describes the system sketched in figure 5.6 with unit cells containing two lattice sites. The second-neighbour hopping can be seen as a perturbation of the previously discussed system.

Again Fourier transform can be applied following the steps obtained in appendix A. The calculation is sketched in the following. In a tensor product basis, in which A and B take on the role of the internal indices of the unit cells labelled with $n$ the Hamiltonian reads

$$H = \sum_{n=1}^{N/2} t_- \left( |n, A \rangle \langle n, B| + \text{h.c.} \right) + t_+ \left( |(n \text{ mod } N/2) + 1, A \rangle \langle n, B| + \text{h.c.} \right)$$

$$+ \frac{i\Gamma}{2} \left( |n, A \rangle \langle n, A| - |n, B \rangle \langle n, B| \right)$$

$$+ t_{2nd} \left( |n, A \rangle \langle (n \text{ mod } N/2) + 1, A| + |n, B \rangle \langle (n \text{ mod } N/2) + 1, B| + \text{h.c.} \right)$$. 

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Figure 5.7.: Ground state expectation values of the occupation number operator for the SSH model with 16 lattice sites with constant second neighbour hopping subject to an alternating imaginary potential $U_{\text{alt}}$ (cf. equation (5.3)) with $t = 1, \Delta = 0.5, \Gamma = 1.4$ and $\theta = \pi/8$ in (a) and (b) respectively $\theta = 7\pi/8$ in (c). The maximal $\mathcal{PT}$-broken ground state in (b) has a 0.1% smaller real part of the complex energy eigenvalue compared to the $\mathcal{PT}$-unbroken ground state in (a).

with periodic boundary conditions. The application of the relations

$$|n\rangle = \frac{1}{\sqrt{N/L}} \sum_{k=-\pi}^{\pi} e^{-i kn} |k\rangle, \quad \delta_{kq} = \frac{1}{N/L} \sum_{n=1}^{N/L} e^{-i n(k-q)}$$

provides the Hamiltonian in the Fourier basis

$$H = \sum_{k=-\pi}^{\pi} \left( t_- + t_+ e^{-i k} \right) |k, B\rangle \langle k, A| + \left( t_- + t_+ e^{i k} \right) |k, A\rangle \langle k, B|$$

$$+ \left( \frac{i \Gamma}{2} + 2t_{\text{2nd}} \cos(k) \right) |k, A\rangle \langle k, A| + \left( -\frac{i \Gamma}{2} + 2t_{\text{2nd}} \cos(k) \right) |k, B\rangle \langle k, B|,$$

from which on reads off the Bloch Hamiltonian

$$\mathcal{H} = \begin{pmatrix} \frac{i \Gamma}{2} & t_- + t_+ e^{-i k} & \frac{i \Gamma}{2} \\ t_- + t_+ e^{i k} & -i \Gamma / 2 & 2t_{\text{2nd}} \cos(k) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$ 

This Bloch Hamiltonian is exactly the same as for the $\mathcal{PT}$-symmetric SSH model with alternating gain and loss, and without second-neighbour hopping, which is discussed above, except for a term proportional to the identity matrix, which does not change its eigenstates. The band gaps and the gap closings of the dispersion relation are not changed significantly. Thus the biorthogonal basis of eigenstates, and therefore the complex Zak phases are the same as in the previous case following from the Bloch Hamiltonian given in equation (5.5). The introduction of second-neighbour hopping does not break the $\mathcal{PT}$ symmetry, which protects the topological phases in the system. The previously found topological phases are therefore stable under this perturbation.

Again the existence of edge states indicates topologically nontrivial behaviour in the parameter regime with a nontrivial real part of the complex Zak phase $\gamma$. The occupation number operator expectation values of ground states of a finite version of the system.
5.1. SSH model

Figure 5.8.: Schematic sketch of unit cells with 7 (a) and 9 (b) lattice sites of the SSH model with tunelling amplitudes $t_-$ and $t_+$ subject to an alternating imaginary potential with a defect in the centre of unit cell (represented by an open circle) analogously to figure 5.1. The unit cells are connected with a hopping amplitude $t_+$. The shaded area in (a) and (b) illustrates the concept of understanding the lattice system as a combination of two different dimerised lattices where each of them is highlighted.

without periodic boundary conditions are depicted in figure 5.7 for parameter values of the topologically distinct phases (cf. figure 5.3). Edge states can be found in the topologically nontrivial phase where $\text{Re}(\gamma) = \pi$. A $\mathcal{PT}$-unbroken state with the smallest eigenvalue is shown in 5.7 (a), and again the degenerate partner state looks as the image of the state shown in (a) reflected at an imagined line at $\langle n \rangle = 0.5$. Several $\mathcal{PT}$-broken states coexist with these states. The maximal $\mathcal{PT}$-broken ground state is shown in (b) and has an approximately 0.1% smaller real part as compared to the energy of the $\mathcal{PT}$-unbroken state shown in (a). In the topologically trivial phase characterised by $\text{Re}(\gamma) = 0$ a $\mathcal{PT}$-unbroken ground state is a Mott insulating state, which is shown in figure 5.7 (c). In this parameter regime the ground state is unique.

Alternating gain and loss with a defect

Weimann et al. [38] experimentally investigated a $\mathcal{PT}$-symmetric photonic lattice consisting of a waveguide array which acts like a one-dimensional PT-symmetric lattice with alternating gain and loss. They created a topological defect by inserting a lattice site with no complex on-site potential into the centre of the alternating gain and loss profile and connected this additional site with the same hopping amplitude to both neighbouring sites. The lattice has an odd number of sites and is schematically sketched in figure 5.8 (where for now the lattices should consist of only one unit cell). Two possible realisations can be found. One in which the edges of the lattice and the defect are coupled by the same hopping amplitude (cf. figure 5.8 (a)) and one in which the edges and the defect are connected with different amplitudes to the neighbouring sites (cf. figure 5.8 (b)). In the case shown in (a) the edges and the defect can host topological states located mainly at a single lattice site in the same parameter regime, while systems of the type shown in (b) host edge states when no topological state is located primarily at the single lattice site of the defect and vice versa. The topological state occurring at the defect
in the centre of the lattice is a topological interface state between two topologically distinct lattices. Therefore, one interprets the lattices to consist of two parts with different dimerisations, which are highlighted by shaded areas in figure 5.8. The part containing the defect in the centre of the lattice has an odd number of lattice sites and always a weakly coupled site at one edge. Hence it should host “edge states” in both dimerisation configurations (θ < π/2 and θ > π/2). The interpretation as a system with a topological interface state indicates topologically nontrivial phases both for θ < π/2 and θ > π/2. Thus the complex Zak phases are expected to show a topologically nontrivial phase in the \( PT \)-unbroken parameter regime for both dimerisation configurations. This is verified by a calculation of the complex Zak phase of this system.

Thus the approach seems promising and lattices built up from unit cells, which have an analogous structure are studied in the following. These systems possess a translational symmetry, and hence a construction of a Bloch Hamiltonian is possible by following the steps in appendix A. The unit cells of the lattices are shown in figure 5.8 and possess either 7 or 9 lattice sites. Thus they are of the two different previously mentioned types. The Bloch Hamiltonian of the first realisation with 7 sites per unit cell is given by

\[
\mathcal{H}_{7\times7} = \begin{pmatrix}
\frac{i\Gamma}{2} & t_- & 0 & 0 & 0 & 0 & t_+ e^{ik} \\
-t_- & -\frac{i\Gamma}{2} & t_+ & 0 & 0 & 0 & 0 \\
0 & t_+ & \frac{i\Gamma}{2} & t_- & 0 & 0 & 0 \\
0 & 0 & t_- & 0 & t_- & 0 & 0 \\
0 & 0 & 0 & t_- & -\frac{i\Gamma}{2} & t_+ & 0 \\
0 & 0 & 0 & 0 & t_+ & \frac{i\Gamma}{2} & t_- \\
t_+ e^{-ik} & 0 & 0 & 0 & 0 & t_- & -\frac{i\Gamma}{2}
\end{pmatrix}
\]

(5.18)

and the one for the realisation with 9 lattice sites per unit cell reads

\[
\mathcal{H}_{9\times9} = \begin{pmatrix}
\frac{i\Gamma}{2} & t_- & 0 & 0 & 0 & 0 & 0 & 0 & t_+ e^{ik} \\
t_- & -\frac{i\Gamma}{2} & t_+ & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & t_+ & \frac{i\Gamma}{2} & t_- & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & t_- & -\frac{i\Gamma}{2} & t_+ & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & t_+ & \frac{i\Gamma}{2} & t_- & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & t_- & -\frac{i\Gamma}{2} & t_+ & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & t_+ & \frac{i\Gamma}{2} & t_- & 0 \\
t_+ e^{-ik} & 0 & 0 & 0 & 0 & 0 & t_- & -\frac{i\Gamma}{2} & 0
\end{pmatrix}
\]

(5.19)

The complex Zak phases following from these two Bloch Hamiltonians are computed by applying the gauge smoothing algorithm presented in chapter 4. The results are shown in figure 5.9 in (a) for the version with 7 sites and in (b) for the realisation with 9 sites per unit cell. Indeed the Zak phases indicate a topologically nontrivial phase in the \( PT \)-unbroken parameter regimes for both systems for θ < π/2 as well as for θ > π/2. The only difference between the two different lattice types is the behaviour of the Zak
Figure 5.9.: Complex Zak phases of the SSH model subject to an alternating imaginary potential with a defect in the unit cell centre in dependence of the dimerisation parameter $\theta$ and the parameter of gain and loss $\Gamma$. The system parameters are $t = 1$ and $\Delta = 1$. Here $\gamma_0$ is the Zak phase corresponding to the eigenvalue branch being always negative for $k = 0$, $\gamma_1$ belongs to the eigenvalue branch being always positive for $k = 0$, respectively. The hatched area marks the $\mathcal{PT}$-broken parameter regime of the corresponding eigenvalues which are shown in figure 5.10 for (b).
5. $\mathcal{PT}$-symmetric lattice systems

The bands are gapped as long as the energies are real-valued and become gapless as $\theta$ is varied from 0 towards $\pi/2$. The band gaps close pairwise at $k = 0$ and $k = \pm \pi$ starting with the central bands. A further increase of the value of $\theta$ beyond $\theta = \pi/2$ leads to a reopening of these band gaps in the reversed order until all energy bands are gapped again in the $\mathcal{PT}$-unbroken regime. The labelling of the energy bands is consistent with the labelling of the complex Zak phases shown in figure 5.9 (b).

phases ($\gamma_0$ and $\gamma_6$ in (a) and $\gamma_0$ and $\gamma_8$ in (b)) corresponding to the energy bands with a minimal and maximal real part of the complex energy. The energy bands corresponding to the Zak phases shown in 5.9 (b) are shown in figure 5.10. The labelling of the energy bands and the complex Zak phases in 5.9 (b) is consistent. For small values of $\theta$ the energy bands are gapped. As one increases $\theta$ towards $\pi/2$ the band gaps close pairwise at $k = \pm \pi$ and $k = 0$ starting with the central band (cf. $E_4$ in figure 5.10). For $\theta = \pi/2$ the spectrum is completely gapless. A further increase of the dimerisation parameter $\theta$ causes the band gaps to reopen in the reversed order until all bands are gapped again and the dispersion looks similar to the one depicted on the left in the top row of figure 5.10 for values of $\theta \approx \pi$.

Also in this case an investigation of the many-body ground states of finite lattice systems substantiates the topologically nontrivial phases of the bulk indicated by a real part of the complex Zak phases of $\pi$. An investigation of the many-body ground states of
finite lattices with 15 and 17 lattice sites shows two different kinds of edge states. Those
which are located at the defect at the interface between the two differently dimerised
lattices and those which are located at the edges of the lattice. The latter behave like
the previously discussed edge states, as they are found in the regime where the sites at
the edges are coupled with a weak tunnelling amplitude to the neighbouring sites.

The lattice with 15 sites is of the same type as the previously discussed lattice with
7 sites (shown in figure 5.8 (a)), as the sites at the edges and the central cite hosting
the defect are coupled with the same hopping amplitude to their neighbouring sites.
Topological states can be identified at the edges and the defect for the same dimerisation
θ < π/2. In this case the edges and the defect are coupled with a weak hopping amplitude
to their neighbouring sites. One finds eight different ground states for θ < π/2 with
the same real part of the complex energy. Four of them are \( \mathcal{PT} \)-broken, where
the other four are \( \mathcal{PT} \)-unbroken. A \( \mathcal{PT} \)-unbroken ground state is shown in figure 5.11 (a)
and the maximal \( \mathcal{PT} \)-broken ground state is shown in 5.11 (b), which has an inverted
occupation at the right edge compared to the state shown in (a). The shapes of all
other \( \mathcal{PT} \)-(un)broken ground states are obtained by all possible reflection antisymmetric
(symmetric) images mirrored at an imagined line at \( \langle n \rangle = 0.5 \) with inverted occupation
at the edges and the defect.

The Zak phases in figure 5.9 (a) indicate the existence of a topologically nontrivial
state in the regime with θ > π/2. In this parameter regime the three sites at the centre
of the lattice are coupled together with a strong hopping amplitude, and form a trimer,
which should host a topological interface state. But the states found in this parameter regime do not allow for a clear interpretation. For $\theta > \pi/2$ two degenerate and $\mathcal{PT}$-symmetric ground states are found. One of them is shown in 5.11 (c), and the other one looks like its reflection image at an imagined line at $\langle n \rangle = 0.5$. These states cannot be interpreted as a topological interface state in an unambiguous way as properties like the exponential decay of the probability density are not visible. An investigation of lattices with significantly more sites could clarify the question whether topological states can be found in the regime with $\theta > \pi/2$ at the interface of the two differently dimerised parts of the lattice.

The same occupation of the sites of the trimer in the centre of the unit cell can be found in the lattice version with 17 sites (cf. 5.11 (d) and (e)), which is of the same type as the system shown in figure 5.8 (b). Here the occupation of the edges occurs for $\theta < \pi/2$, whereas the defect has a protruding occupation for $\theta > \pi/2$ (cf. 5.11 (f)). Again eight different ground states appear for $\theta < \pi/2$, four $\mathcal{PT}$-unbroken and four $\mathcal{PT}$-broken states. Two of them are shown, a $\mathcal{PT}$-unbroken ground state in (d) and the maximal $\mathcal{PT}$-broken ground state in (e). The shapes of all other $\mathcal{PT}$-(un)broken ground states are again obtained by all possible reflection antisymmetric (symmetric) mirror images of the occupations at the edges and the trimer in the centre of the lattice at an imagined line at $\langle n \rangle = 0.5$. In the system with 17 sites the defect is coupled with a weak hopping amplitude to the neighbouring sites for values of $\theta > \pi/2$. In this regime a topological interface state can be found, which is similar to the one at the defect in the lattice with 15 sites for $\theta < \pi/2$ (cf. 5.11 (a) and (b)) and has a localised occupation probability at the single lattice site hosting the defect.

5.1.2. Unit cells with gain and loss at their edges

In the following the SSH model with gain and loss located at the edges of each unit cell is investigated. Hereby, $L$ is the number of lattice sites per unit cell and only even numbers $L > 2$ are taken into account, such that the sites at the edges are always coupled via a tunnelling amplitude $t_-$ to the neighbouring lattice site of the same unit cell and with $t_+$ to the edge of the neighbouring unit cell. A complex potential describing gain and
loss at the edges of the unit cells on a lattice with a total number of \( N \) sites is given by

\[
U_{\text{edge}} = \frac{N}{L} \sum_{n=1}^{N/L} \left( c_{L(n-1)}^{\dagger} c_{L(n-1)} - c_{L(n-1)-1}^{\dagger} c_{L(n-1)-1} \right),
\]

with periodic boundary conditions which are realised by identifying \( 0 \equiv N - 1 \). A unit cell of the system is illustrated in figure 5.12. The total system is described by the Hamiltonian \( \mathcal{H} = \mathcal{H}_{\text{SSH}} + U_{\text{edge}} \). The eigenstates and eigenvalues of a finite version of this system consisting of one unit cell are studied in [60] using a one-particle basis.

To calculate the complex Zak phases of this system, one sets up the Bloch Hamiltonian by following the steps characterised in appendix A,

\[
\mathcal{H} = \begin{pmatrix}
\frac{i \Gamma}{2} & t_- & 0 & t_+ e^{ik} \\
t_- & 0 & t_+ & \cdots \\
0 & t_+ & \ddots & t_- \\
\cdots & \ddots & \ddots & \cdots \\
t_+ e^{-ik} & \cdots & 0 & t_- \\
t_- & \cdots & t_- & \frac{i \Gamma}{2}
\end{pmatrix}
\] (5.21)

and applies the gauge smoothing algorithm. The numerical integration of the gauge smoothed Berry connection yields the complex Zak phases shown in figure 5.13 for a system built up from unit cells with 20 lattice sites, which is described by a 20 \( \times \) 20 Bloch Hamiltonian. The complex Zak phases can be arranged pairwise with pairs of \( \pm \gamma \). Only two of the complex Zak phases (\( \gamma_4 \) and \( \gamma_6 \)) indicate topological nontrivial behaviour. Again one finds a topologically nontrivial phase for \( \theta < \pi/2 \), but here no statements for small values of \( \Gamma \rightarrow 0 \) can be made as the Bloch Hamiltonian is \( \mathcal{P}\mathcal{T} \)-broken.

The complex dispersion relation of this system is shown in figure 5.14 for different values of the dimerisation parameter \( \theta \). The energy bands corresponding to \( \gamma_4 \) and \( \gamma_6 \) are highlighted. In the \( \mathcal{P}\mathcal{T} \)-unbroken parameter regime of \( \gamma_4 \) and \( \gamma_6 \) the corresponding energy bands \( E_4 \) and \( E_6 \) are gapped. The band gap closes at the \( \mathcal{P}\mathcal{T} \) phase transition, but a gap between the states \( E_4 \) and \( E_6 \) still exists. This band gap closes for a value of \( \theta \) in the \( \mathcal{P}\mathcal{T} \)-broken regime (see figure 5.14 on the left in the second row). For values of \( \theta > \pi/2 \) in the \( \mathcal{P}\mathcal{T} \)-unbroken parameter regime of \( \gamma_4 \) and \( \gamma_6 \) the bands \( E_4 \) and \( E_6 \) are gapped again. The SSH model with gain and loss at the edges of the unit cells shows a particular feature for non-Hermitian systems. The increase of only one parameter causes two \( \mathcal{P}\mathcal{T} \) phase transitions (cf. \( \gamma_4 \) or \( \gamma_6 \) in figure 5.13), even though the system has no periodic dependency of this parameter. The eigenvalues corresponding to \( \gamma_4 \) and \( \gamma_6 \) are complex for small and large values of the parameter of gain and loss \( \Gamma \) but real valued for values of \( \Gamma \) in between. Also the increase of \( \theta \) from zero to \( \pi \) causes two \( \mathcal{P}\mathcal{T} \) phase transitions, but the system depends periodically on this parameter.
The hatched areas mark the \( \mathcal{PT} \)-broken parameter regimes of the eigenvalue corresponding to each Zak phase. Only the Zak phases \( \gamma_4 \) and \( \gamma_6 \) show a topologically nontrivial phase (green areas). A peculiarity of the two eigenvalues corresponding to these Zak phases is the existence of a parameter regime, in which the increase of the parameter \( \Gamma \) causes the \( \mathcal{PT} \)-broken eigenvalues to become real-valued, and a further increase leads to another \( \mathcal{PT} \) phase transition and complex eigenvalues.
5.1. SSH model

Figure 5.14.: Complex dispersion relation of the SSH model with gain and loss at the edges of the unit cells described by $U_{\text{edge}}$ and system parameters $t = 1.0$, $\Delta = 0.5$, $\gamma = 2$, and $\theta$ given in the top the figures. The energies $E_4$ and $E_6$ are highlighted in orange and green (solid line for their real part and a dashed line for their imaginary part). All other energies are represented by solid lines, a blue one for the real part and a red one for their imaginary part. The Zak phases of these two energy bands are topologically nontrivial in a region of the investigated parameter space (cf. figure 5.13). In the $\mathcal{PT}$-unbroken regime of these bands they are gapped (cf. $\theta = 1/16\pi$, $3/8\pi$ and $15/16\pi$). Between $\theta = 3/8\pi$ and $\theta = 25/64\pi$ the two bands become gapless as the gap closes at $k = \pm\pi$, but the band gap between $E_4$ and $E_6$ is still present. This band gap closes at a value of $\theta$ between $\theta = 27/64\pi$ and $\theta = 7/16\pi$ at $k = 0$. A further increase of the value of $\theta$ leads to a reopening of these band gaps until the energy bands $E_4$ and $E_6$ are gapped again in the $\mathcal{PT}$-symmetric and topologically trivial phase (cf. figure 5.13). An exemplary complex dispersion relation in this parameter regime is shown for $\theta = 15/16\pi$.

The same computations can be made for a lattice system with unit cells containing 50 lattice sites. The Bloch Hamiltonian is a $50 \times 50$ matrix of the form given in equation (5.21). Again, one finds only one pair of Zak phases indicating topologically nontrivial phases. These two complex Zak phases are depicted in figure 5.15. One observes the same behaviour as in the case with 20 lattice sites per unit cell, but the $\mathcal{PT}$-unbroken regime is expanded to smaller values of $\Gamma$. On the right hand side of figure 5.15 one
Figure 5.15.: Complex Zak phases in dependency of the dimerisation parameter $\theta$ and the parameter of gain and loss $\Gamma$. The underlying SSH model is subject to an imaginary potential with particle gain on one end of the unit cell and particle loss on the other end. The unit cells comprise 50 lattice sites and the system parameters are $t = 1$ and $\Delta = 0.5$. The hatched areas mark the $\mathcal{PT}$-broken parameter regime, for which the energy eigenvalues corresponding to the eigenstates used to calculate the Zak phase have a nonvanishing imaginary part somewhere in the first Brillouin zone.

can see some numerical noise disturbing the complex Zak phase, resulting from a wrong ordering of the eigenvalue branches as they are located closely to one another and the sorting of the single energy bands breaks down.

To substantiate the topologically nontrivial phases found by the numerical investigation of the complex Zak phase, the many-body ground states of a finite version of this model with 16 lattice sites are studied in the following, again by exact diagonalisation of the many-body Hamiltonian. For parameter values in the topologically nontrivial phase indicated by $\gamma_4$ and $\gamma_6$ in figure 5.13 and $\gamma_0$ and $\gamma_1$ in figure 5.15, the $\mathcal{PT}$-unbroken degenerate many-body ground states are edge states. One of them has the occupation number operator expectation values which are shown in figure 5.16 (a). The other one looks again like the image of the state shown in (a) reflected at an imagined line at $\langle n \rangle = 0.5$. The maximal $\mathcal{PT}$-broken ground state is shown in (b). Its energy eigenvalue has the same real part as the $\mathcal{PT}$-unbroken ground states. In the topologically trivial phase the unique ground state is a Mott insulating state (cf. figure 5.16 (c)) with no striking edge occupation and a 10% smaller energy as the degenerate first excited maximal $\mathcal{PT}$-broken states in (cf. (d) and (e)). This supports the numerical results of the Zak phase.

The maximal $\mathcal{PT}$-broken states (cf. 5.16 (d) and (e)) and especially the second excited maximal $\mathcal{PT}$-broken state, shown in figure 5.16 (f) (which has an energy eigenvalue with an approximately 10% bigger real part and an imaginary part, which is two times greater
5.1. SSH model

Figure 5.16.: Expectation values of the occupation number operator of specific states of the SSH model with 16 lattice sites per unit cell subject to $U_{\text{edge}}$ (cf. equation (5.20)) with $t = 1$, $\Delta = 0.5$, $\Gamma = 1.5$ and $\theta = \pi/8$ in (a) and (b) respectively $\theta = 7\pi/8$ in (c)-(f). The $\mathcal{PT}$-unbroken ground state in (a) and, maximal $\mathcal{PT}$-broken ground state in (b) possess the same real part of the complex energy eigenvalue, whereas the $\mathcal{PT}$-unbroken ground state (c) has a significantly (approximately 10%) smaller real energy as the degenerate first exited maximal $\mathcal{PT}$-broken states in (d) and (e). In (f) the second excited maximal $\mathcal{PT}$-broken state is shown. The real part of the complex energy is approximately 10% bigger than the real part of the maximal $\mathcal{PT}$-broken ground states shown in (d) and (e).

as compared to the states in (d) and (e)) show an interesting behaviour in the regime $\theta > \pi/2$ with strong tunnelling amplitudes coupling the edges to the neighbouring states. The edges are almost completely filled or emptied due to the action of the complex potential. Because of the edges being coupled via strong tunnelling amplitudes to the neighbouring sites, these sites are filled or emptied as well. A dynamical investigation of the steady states of an analogous system (cf. section 6.3.2) reproduces the states in (b) and (f). Thus, in the topologically trivial phase the subsystem, in which the sites at the edges (which are coupled to the reservoir respectively carry the complex potential in an effective non-Hermitian description of this open lattice system) are removed by attributing them to the reservoir, has edges coupled via a weak tunnelling amplitude to the neighbouring sites and is in a topologically nontrivial phase. In the topologically trivial phase the steady state respectively the corresponding dominant state in a unitary-like time evolution reproduces the steady state respectively the dominant state, which occurs in the corresponding smaller system. This gives rise to the presumption that the application of gain and loss at the edges of a dimerised lattice allows for the active preparation of the system in a state of the form shown in 5.16 (b) independently of the dimerisation of the lattice, as in a topologically trivial phase the sites at the edge of the system can be attributed to the reservoir.

The maximal $\mathcal{PT}$-broken states are found to reproduce the occupation number operator expectation values of the steady state, which are found in the course of a dynamical
investigation of analogous open quantum systems. This will be part of the discussion in chapter 6.

Analogous $\mathcal{PT}$-symmetric potentials can be investigated providing similar results. For example the system depicted in figure 5.17 has also a pair of complex Zak phases, which indicate a topologically nontrivial phase in a $\mathcal{PT}$-unbroken regime for $\theta < \pi/2$ and topologically trivial phase in a $\mathcal{PT}$-broken regime for $\theta > \pi/2$. An investigation of the steady states and maximal $\mathcal{PT}$-broken states of this system can be found in [61], which contains also an investigation of the parameter dependence of these states in the systems discussed above.

### 5.2. Kitaev chain

The Hamiltonian describing the one-dimensional Hermitian Kitaev chain with a total number of $N$ sites is given by

$$H = \sum_{n=1}^{N} \mu c_n^\dagger c_n + t \left( c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1} \right) - i\Delta \left( c_n c_{n+1} - c_n^\dagger c_{n+1}^\dagger \right)$$

(5.22)

with fermionic creation and annihilation operators, the chemical potential $\mu$, an homogeneous hopping amplitude $t$ and the so-called p-wave coupling amplitude $\Delta$. The detection of $\mathcal{PT}$-unbroken phases in non-Hermitian extensions of the Kiatev model [45] turns out to be more sophisticated as the $\mathcal{PT}$ symmetry of their Bloch Hamiltonian is found to be broken for all values of $\Gamma \neq 0$. Therefore the quantisation argument of the real part of the complex Zak phase given in section 3.2.1 does not apply and an investigation of the topology of the band structure using the same tools as in the previous part seems to be appropriate on the first sight. Nevertheless, quantised complex Zak phases can be found as the following discussion will show.

#### 5.2.1. Alternating gain and loss

If one subjects the lattice described by equation (5.22) to the alternating complex potential from equation (5.3) (cf. figure 5.18), the resulting Bloch Hamiltonian is given by
5.2. Kitaev chain

Shapes:

\[
\begin{array}{cccc}
\Delta & \Delta & \Delta & \Delta \\
\end{array}
\]

Figure 5.18.: Schematic sketch of a unit cell of the Kitaev chain with a real on-site potential $\mu$ tunnelling amplitudes $t$ and a p-wave coupling amplitude subject to an alternating imaginary potential.

\[
\mathcal{H} = \begin{pmatrix}
-\mu - 2t \cos(k) & -2\Delta \sin(k) & 0 & -i\gamma/2 \\
-2\Delta \sin(k) & \mu + 2t \cos(k) & i\gamma/2 & 0 \\
0 & i\gamma/2 & \mu - 2t \cos(k) & 2\Delta \sin(k) \\
-i\gamma/2 & 0 & 2\Delta \sin(k) & -\mu + 2t \cos(k)
\end{pmatrix},
\]

(5.23)

where the Hamiltonian results from this matrix by a representation in the spinor decomposition $H = \sum_{k=0}^{\pi/2} (c_k, c_k^\dagger, c_{\pi-k}, c_{\pi-k}^\dagger) \mathcal{H}(c_k^\dagger, c_{-k}, c_{\pi-k}, c_{\pi-k}^\dagger)^T$. As the lattice is built up from unit cells comprising two lattice sites, but the p-wave coupling term has to be included in the matrix representation, the sum runs just form 0 to $\pi/2$ and the dispersion relation has a periodicity of $\pi$, which can be seen in figure 5.19. This figure additionally illustrates that the Bloch Hamiltonian is $\mathcal{PT}$-broken as no real energy bands can be found.

Thus, the $\mathcal{PT}$-symmetry of the Bloch Hamiltonian from equation (5.23) is broken. This holds for all values $\Gamma \neq 0$, even though the imaginary part of the eigenvalues would become arbitrary small for $\Gamma \to 0$. In the weak non-Hermitian regime (which is obviously given for $\Gamma \neq 0$ as the magnitude of the imaginary energy eigenvalue is of the same order as the adiabatic slowness parameter in the derivation of the complex Berry phase) the Berry phase is well defined [57, 62]. Therefore one presumes that the $\mathcal{PT}$-symmetric complex potential acts like a perturbation in this regime and proceeds with the investigations in the same procedure as in the case of the SSH model. Because of the different choice of the basis of the Bloch Hamiltonian (see below equation (5.23)), the loop in parameter space is of a different kind as in the previous discourse. Here $k$ is varied from $-\pi/2$ to $\pi/2$ to close a loop in parameter space and the eigenstates of the Bloch Hamiltonian do not need to be single valued as in the previous discussion, rather each eigenvector must be the constant continuation of another under variation above the border $-\pi/2$.

If one applies the numerical method from chapter 4 to the Bloch Hamiltonian from equation (5.23) and uses a loop parametrised by $k$ and varied from $-\pi/2$ to $\pi/2$, one obtains the complex Zak phases shown in figure 5.20. The imaginary parts of the Zak phases turn out to be zero. Two of them ($\gamma_1$ and $\gamma_2$) indicate topologically nontrivial phases. The corresponding energy bands are shown in figure 5.19 for different values of the chemical potential $\mu$. If one increases $\mu$ starting from a value of $-3$ a band gap closing (between the real and imaginary part of $E_1$ and $E_2$) can be found around the value $\mu = -1.5$. At this point the topology changes (see $\gamma_1$ and $\gamma_2$ in figure 5.20). Thus, even though the imaginary part of the energy eigenvalues
Figure 5.19.: Complex dispersion relation of the Kitaev model subject to an alternating complex potential obtained from the Bloch Hamiltonian given in equation (5.23) with system parameters $\Delta = 0.25$, $t = 0.5$, $\mu = 0.75$ and the values of $\Gamma$ given above the graphs. The $\mathcal{PT}$ symmetry of the Bloch Hamiltonian is broken for all values of $\Gamma \neq 0$, even though the imaginary part of the eigenvalues gets arbitrarily small for $\Gamma \to 0$.

are assuredly not of the same magnitude as the adiabatic slowness parameter in the derivation of the complex Berry phase, the numerically computed complex Zak phases seem to be promising. Indeed the results of investigation of the energy spectrum and the states of a finite version of the same model indicate the occurrence of a topological nontrivial phase in the same parameter regime of this system [19].

Thus, the complex Zak phase (which is the first order approximation of the coefficients given by equation (3.16)) seems to be of significance even in the $\mathcal{PT}$-broken parameter regime. The algorithm (see figure 4.2) provides an universal tool for the calculation of complex Berry phases in various systems.

5.2.2. Particle loss

As the need of real eigenvalues seems not to be a restrictive condition for the detection of topologically nontrivial phases using the complex Zak phase as topological invariant, a non-Hermitian, non-$\mathcal{PT}$-symmetric system is investigated in the following. It is described by the Hamiltonian $H + U_{\text{loss}}$ with $H$ from equation (5.22) and a complex
5.2. Kitaev chain

\[ U_{\text{loss}} = \sum_{n=1}^{N} -i\Gamma . \] (5.24)

This system is illustrated in figure 5.21 and a Fourier transform leads to a Bloch Hamiltonian of the form

\[ \mathcal{H} = \begin{pmatrix} t \cos(k) + \mu/2 - i\gamma/2 & 2\Delta \sin(k) \\ 2\Delta \sin(k) & -t \cos(k) - \mu/2 + i\gamma \end{pmatrix}, \] (5.25)

where here the spinor basis

\[ H = \sum_{k=0}^{\pi} (c_k, c_k^\dagger) \mathcal{H} \begin{pmatrix} c_k^\dagger \\ c_{-k} \end{pmatrix} \] (5.26)

was used to represent the Bloch Hamiltonian. From which one can see the particle-hole (or charge conjugation) symmetry \( \mathcal{C} \), as well as the reflection (\( \mathcal{P} \)) and time inversion symmetry (\( \mathcal{T} \)) of the system for \( \Gamma = 0 \). For values \( \Gamma \neq 0 \) these symmetries are broken, but in this case the system is again invariant under the combined action of all these symmetry operations,

\[ [\mathcal{H}, \mathcal{CPT}] = 0 , \] (5.27)

which can be illustratively explained by thinking of the action of all these symmetry operations. The time reversal symmetry \( \mathcal{T} \) reverses the imaginary potential on each site,
the parity operator $\mathcal{P}$ spatially inverts the lattice and the charge conjugation operator changes the creators and annihlitors of fermions into annihlitors and creators of holes, for which the gain of particles on each lattice site acts as a complex potential describing the loss of holes on each site. Therefore, the symmetry inverted system describes a Kitaev chain of holes with loss on each site of the lattice, and thus $CPT$ is a symmetry of the system.

The application of the numerical method on the Bloch Hamiltonian, given by equation (5.25), with a loop in parameter space parametrised by $k$ running from $-\pi$ to $\pi$. Although the eigenvalues of this model are complex for all $\Gamma \neq 0$, the complex Zak phase is quantised. The antiunitary symmetry applying to the quantisation argument of Hatsugai [58] is the $CPT$ symmetry. The Zak phases of the model are shown in figure 5.22. One finds a topologically nontrivial phase with $\text{Re}(\gamma) = \pi$, which is in accordance with the investigations of this system found in [63] (page 54 ff.), in which a condition for the topological phase transition was derived,

$$
\Gamma^2 + \frac{\mu}{4} = t^2.
$$

This relation is plotted with a red dashed line in figure 5.22. Again an excellent agreement between the results can be found.

**Remarks**

In summary of this chapter one can see that topological phases exist in one-dimensional $\mathcal{PT}$-unbroken lattice systems, which can be classified by the real part of the complex Zak phase, even if the Hamiltonian does not possess a chiral symmetry (e.g. the Bloch Hamiltonian given by equation (5.5)), which is often used to show the quantisation of the bulk winding number. Further, the many-body ground states found in finite versions of the $\mathcal{PT}$-symmetric lattice systems show the same characteristic edge features as in the Hermitian versions of the models. This substantiates the characterisation of the topological phases by the complex Zak phase. The application of the algorithm (see figure 4.2) on $\mathcal{PT}$-symmetric versions of the Kitaev chain shows its versatility. Even though the eigenvalues are complex and the $\mathcal{PT}$ symmetry of the system is broken one can use numerical method as a tool to investigate the topological phases of the system. The numerical method is a powerful tool to investigate the topology of various lattice
5.2. Kitaev chain

Figure 5.22.: Complex Zak phases of the Kitaev model subject to an imaginary potential with particle loss of the same strength on every lattice site. The model is inversion symmetric and the system parameters are \( t = 1 \) and \( \Delta = 0.5 \). The energy eigenvalues corresponding to the eigenstates used to calculate the Zak phase have a nonvanishing imaginary part somewhere in the first Brillouin zone for every \( \Gamma \neq 0 \). The dashed red line marks the phase transition according to equation (5.28) [63].

systems. This will become even clearer, in the next chapter in which the algorithm is applied on dissipative systems described by Lindblad master equations.
6. Lindblad description of open lattice systems

The first part of this chapter provides an introduction to master equations in Lindblad form. In this context Bardyn et al. [15] investigated topological properties of open quantum systems. They compared the Liouvillian case to the Hamiltonian scenario and defined topologically ordered states as “locally indistinguishable steady states of a gapped quantum many-body Liouvillian with a dissipative gap and a purity gap” and a winding number as a corresponding topological invariant for one-dimensional systems.

In section 6.2 the formalism of third quantisation is introduced, by following the work of Prosen [43], which provides a tool to compute steady states of the dissipative dynamics of an open quantum system. In analogy to the Hamiltonian band theory of closed and open lattice systems with a translational symmetry, effectively described by a non-Hermitian \( \mathcal{PT} \)-symmetric theory (see chapter 5), a Fourier transform can be applied [15, 43] to the Liouvillian resulting in a non-Hermitian matrix, which is comparable to the Bloch Hamiltonian and therefore is called Bloch Liouvillian in the following. By driving this analogy further, a phase can be constructed from the left and right handed eigenvectors of the Bloch Liouvillian, which is analogous to the Zak phase investigated in the previous parts of this thesis. This phase is called dissipative Zak phase in the scope of this work. In this context, the algorithm from chapter 4 is able to demonstrate its strengths as the eigenvalues of the Bloch Liouvillian are complex and the determination of gauge smoothed eigenvectors is mandatory for a numerical computation of the dissipative Zak phase. The aim of this chapter is to obtain a topological invariant from a numerical instigation, that characterises the steady state of a given dissipative system in analogy to the topological classification of Bloch bands, by using the dissipative Zak phase, which classify the bands of the Bloch Liouvillian.

6.1. Lindblad master equations

This section is based on the discussion of Lindblad master equations in [64]. An open quantum system can be described as a system which interacts with its environment. The full system, which is the combination of the embedded system and its environment, is a closed system. In most cases the observables acting on the Hilbert space of the system are of interest and the observables of the environment are of minor relevance. Therefore it is convenient to divide the Hilbert space of an open quantum system into that of the
system and that of the environment, so that the Hamiltonian of the total system can be written as
\[ \hat{H} = H_S \otimes I_E + I_S \otimes H_E + \hat{H}_I , \]  
(6.1)
where \( I \) is the identity operator, the interaction between the environment and the system is described by \( \hat{H}_I \), the operators labelled with \( S \) act on the Hilbert space of the system, those labelled with \( E \) act on the Hilbert space of the environment, and the superscripted \( \sim \) labels operators acting on the whole Hilbert space. The expectation value of an observable acting on the Hilbert space of the system \( \hat{A} = A_S \otimes I_E \) can be expressed as
\[ \langle \hat{A} \rangle = \text{tr} \left( (A_S \otimes I_E) \hat{\rho} \right) = \text{tr}_S \left( A_S \text{tr}_E (\hat{\rho}) \right) = \text{tr}_S \left( A_S \rho_S \right) \]  
(6.2)
with the partial traces over the system and the environment \( \text{tr}_S \) and \( \text{tr}_E \) and the reduced density matrix of the system
\[ \rho_S = \text{tr}_E (\hat{\rho}) . \]  
(6.3)
Therefore, an equation for the time evolution of the system can be obtained by applying the partial trace over the environment variables on the Liouville-von Neumann equation of the full system (system and environment),
\[ \frac{d}{dt} \rho_S = -i \frac{\hbar}{\hbar} \text{tr}_E \left[ \hat{H}, \hat{\rho} \right] . \]  
(6.4)
Here a decomposition of the interaction Hamiltonian into a tensor product of operators acting on the system and environment
\[ \hat{H}_I = \sum_\kappa = H_{I_{S,\kappa} \otimes H_{I_{E,\kappa}}} , \]  
(6.5)
is assumed to exist, enabling the calculation of the partial trace on the right hand side of equation (6.4). To obtain the Lindblad master equation, one applies the following approximations and assumptions.

At first, one assumes that the system is not correlated with the environment at an initial point of time \( t = 0 \), and therefore the states of the complete system are separable and can be written as
\[ \hat{\rho}(0) = \rho_S(0) \otimes \rho_E(0) . \]  
(6.6)
In a second step the Born approximation is applied, which assumes week coupling between the system and its environment, such that the dynamics of the environment does not influence the evolution of the system. Thus, a state of the complete system can always be written as
\[ \hat{\rho}(t) = \rho_S(t) \otimes \rho_E . \]  
(6.7)
The third approximation is known as Markov approximation, which states that any correlation in the environment decays on a much shorter timescale as correlations decay in the system, i.e.
\[ \tau_E \ll \tau_S \]  
(6.8)
6.2. Third quantisation

with the correlation times of the system $\tau_S$ and the environment $\tau_E$.

The last step is to apply the secular approximation, which is the quantum master equation analogue of the rotating wave approximation.

The application of all these approximations yields the master equation in Lindblad form [65],

$$\frac{d}{dt}\rho_S = \mathcal{L} \rho_S := -\frac{i}{\hbar}[H_S, \rho_S] + \sum_{\mu} \left( L_{\mu}\rho_S L_{\mu}^\dagger - \frac{1}{2} L_{\mu}^\dagger L_{\mu}\rho_S - \frac{1}{2}\rho_S L_{\mu}^\dagger L_{\mu} \right). \quad (6.9)$$

Here dissipation is described by the Lindblad operators $L_{\mu}$, which are arbitrary operators characterising the coupling of a lattice site $\mu$ to a bath or reservoir. For localized single-particle gain (g) and loss (l) they are $L_{g_j} = c_j^\dagger$ and $L_{l_j} = c_j$. In the following the indices (S) are dropped in the notation.

6.2. Third quantisation

The following section yields an introduction to the framework of third quantisation as a method to solve master equations for fermionic quadratic dissipative systems based on the work of T. Prosen [43], where another convention for the Lindblad master equation is used (see equation (6.19)). In the following, the reduced Planck constant is set to one in the notation, $\hbar = 1$.

Starting point is the Lindblad master equation, where the Hermitian Hamiltonian is expressed in a basis of Majorana operators $w_j = w_j^\dagger$,

$$w_{2m-1} = c_m + c_m^\dagger, \quad w_{2m} = i(c_m - c_m^\dagger), \quad (6.10)$$

which fulfill the anticommutation relation

$$\{ w_j, w_p \} = 2\delta_{jp} \quad (6.11)$$

for $m = 1, 2, ..., N$ and $j, p = 1, 2, ..., 2N$ with the number of fermions $N$ and fermionic creation and annihilation operators $c_m^\dagger$ and $c_m$. The Hamiltonian expressed in the basis of these Majorana operators reads

$$H = \sum_{j,p=1}^{2N} w_j H_{jp} w_p = w^T \mathbf{H} w \quad (6.12)$$

and can always be chosen as an antisymmetric matrix, as the Hermitian Majorana operators generate a Clifford algebra, $\mathbf{H} = -\mathbf{H}^T$. In this basis the linear Lindblad operators modelling the dissipation are given

$$L_{\mu} = \sum_{j=1}^{2N} l_{\mu,j} w_j = l_{\mu} \cdot w. \quad (6.13)$$
In the following, \( x^T = (x_1, ..., x_p, ...)^T \) will label a vector of symbols \( x_p \) (scalar valued or operators). The linear \( 2^{2N} = 4^N \) dimensional space \( \mathcal{K} \) of operators \( w_j \) has a Hilbert space structure and a canonical basis,

\[
|P_\alpha\rangle = |P_{\alpha_1, \alpha_2, ..., \alpha_{2N}}\rangle = |w_1^{\alpha_1} w_2^{\alpha_2} ... w_{2N}^{\alpha_{2N}}\rangle \tag{6.14}
\]

with \( \alpha_j \in \{0, 1\} \). This canonical basis is orthonormal with respect to the inner product \( \langle x|y \rangle = 4^{-n}\text{tr}(x^\dagger y) \), which can been seen when one considers the trace of a fermionic creation or annihilation operator on a Fock state,

\[
\langle ..., 1, ... | c_m | ..., 1, ... \rangle = 0 , \\
\langle ..., 0, ... | c_m | ..., 0, ... \rangle = 0 , \\
\langle ..., 0, ... | c_m^\dagger | ..., 0, ... \rangle = 0 , \\
\langle ..., 1, ... | c_m | ..., 1, ... \rangle = 0 , \tag{6.15}
\]

and bears in mind the definition of the Majorana operators in equation (6.10) such that \( \text{tr}(\langle P_\alpha|P_\alpha^\dagger \rangle) = 0 \) if not all \( \alpha_j = \alpha_j' \). From equation (6.14) one sees \( \text{tr}(\langle P_\alpha|P_\alpha^\dagger \rangle) = 4^n \) because \( w_j^2 = 1 \). Due to its form, the canonical basis can be interpreted as orthonormal vectors in a Fock space. One can define a set of linear maps \( \hat{c}_j \) acting on the canonical basis states analogously to annihilators on a Fock state,

\[
\hat{c}_j |P_\alpha\rangle = \delta_{\alpha, 1} |w_j P_\alpha\rangle \tag{6.16}
\]

with \( j = 1, 2, ..., 2N \) and the superscripted \( ^\dagger \) labels linear maps over \( \mathcal{K} \). Then, the adjoint linear maps \( \hat{c}_j^\dagger \) act on the canonical basis states analogously to creators on a Fock state,

\[
\langle P_\alpha|\hat{c}_j^\dagger |P_\alpha\rangle = \langle P_\alpha|\hat{c}_j |P_\alpha^\dagger \rangle = \delta_{\alpha, 1} \langle P_\alpha|w_j P_\alpha^\dagger \rangle = \delta_{\alpha, 0} \langle P_\alpha|w_j P_\alpha \rangle \tag{6.17}
\]

where the orthogonality of the canonical states was used to obtain the last equality. These linear maps over \( \mathcal{K} \) fulfil fermionic commutation relations,

\[
\{\hat{c}_j, \hat{c}_p^\dagger\} = 0 , \quad \{\hat{c}_j, \hat{c}_p\} = \delta_{jp} , \tag{6.18}
\]

for \( j, p = 1, 2, ..., 2N \). One can express the Liouville map \( \mathcal{L} \) occurring in equation (6.9) with \( H \) defined by equation (6.12) and \( L \) defined by equation (6.13) as quadratic form in \( \hat{c}_j \) and \( \hat{c}_j^\dagger \) such that it is a map over \( \mathcal{K} \) which is denoted as \( \hat{\mathcal{L}} \). To do so, one splits the Liouville map \( \hat{\mathcal{L}} \) in an unitary part and a dissipative part,

\[
\hat{\mathcal{L}} \rho \equiv -i[H, \rho] + \sum_\mu \left( 2L_\mu \rho L_\mu^\dagger - \{L_\mu^\dagger L_\mu, \rho \} \right) , \tag{6.19}
\]

\( \hat{\mathcal{L}}_0 \) (unitary) \( \hat{\mathcal{L}}_\mu \) (dissipative)
where the subscript $S$ (system) has been dropped. One can think of the space $\mathcal{K}$ being spanned by all possible pure one-particle density matrices of the system expressed by $|P_\alpha\rangle$. Thus, the unitary part of the Liouville map $\hat{L}_0$ contains terms in which all possible commutators of $w_j w_p$ and elements of $\mathcal{K}$ occur. To keep the proceeding understandable, a commutator of $w_j w_p$ with a canonical basis vector $P_\alpha$ is calculated as an example in the following,

$$|w_j w_p P_\alpha\rangle - |P_\alpha w_j w_p\rangle = 2\left(\delta_{\alpha_1 j} \delta_{\alpha_0 0} + \delta_{\alpha_0 j} \delta_{\alpha_1 0}\right) |P_\alpha\rangle$$

$$= 2\left(\hat{c}_j^\dagger \hat{c}_p - \hat{c}_p^\dagger \hat{c}_j\right) |P_\alpha\rangle . \tag{6.20}$$

As $\mathcal{K}$ is a linear space, an arbitrary element can be decomposed in terms similar to equation (6.20), and the unitary part of the Liouvillean resulting from an arbitrary quadratic Hamiltonian can be expressed as

$$\hat{L}_0 = -4i \left(\hat{c}\right)^T H \hat{c}. \tag{6.21}$$

The dissipative part $\hat{L}_\mu$ can be expressed similarly in the basis of Fermi maps $\hat{c}$ and $\hat{c}^\dagger$. To this end one applies $\hat{L}_\mu$ on the density matrix $\rho$,

$$\hat{L}_\mu \rho = 2L_\mu \rho L_\mu^\dagger - \left\{ L_\mu^\dagger L_\mu, \rho \right\} = \sum_{j,p=2n}^{2n} l_{\mu,j}^* l_{\mu,p} \hat{L}_{jp} \rho \tag{6.22}$$

with $\hat{L}_{jp} \rho = 2w_j \rho w_p - w_p \rho w_j - \rho w_p w_j$, and calculates the action of $\hat{L}_{jp}$ on the vectors of the canonical basis of the space $\mathcal{K}$. Note that the commutation behaviour of $P_\alpha$ and $w_j$ depends only on the magnitude of the vector $\alpha$ and its $j$-th component,

$$P_\alpha w_j = (-1)^{|\alpha|+\alpha_j} w_j P_\alpha , \tag{6.23}$$

and therefore

$$\hat{L}_{jp} |P_\alpha\rangle = \left[2 (-1)^{|\alpha|+\alpha_j} w_j w_p - w_p w_j - (-1)^{|\alpha_j|+\alpha_p} w_p w_j\right] |P_\alpha\rangle . \tag{6.24}$$

The operator space $\mathcal{K}$ is spanned by all $|P_\alpha\rangle$ but the Hamiltonian and the Liouville map $\hat{L}_\mu$ contain only quadratic terms in the operators $w_j$. Consequently, the subspace with $|\alpha|$ contains all relevant states. The unitary part conserves the magnitude of $\alpha$, which can be seen when one defines a number operator in the operator space $\mathcal{K}$,

$$\hat{N} = (\hat{c})^T \cdot \hat{c} = \sum_{j=1}^{2n} \hat{c}_j^\dagger \hat{c}_j , \tag{6.25}$$

and calculates the commutator $[\hat{L}_0, \hat{N}] = 0$. In contrast, the dissipative part of the Liouvillian is not commutating with the number operator $\hat{N}$.
The operator space $\mathcal{K}$ can be decomposed into a direct sum of an even and odd operator space with respect to the parity operator $\hat{P} = \exp(i\pi N)$,

$$\mathcal{K} = \mathcal{K}^+ \oplus \mathcal{K}^- \ . \quad (6.26)$$

Because of this, both the unitary and the dissipative part of the Liouvillian commute with $\hat{P}$ and conserve the parity. The statement is trivial for the unitary part because it commutes with the number operator $[\hat{L}_0, N] = 0$. The dissipative part (cf. equation (6.24)) can be written as

$$\hat{L}_{jp} = (1 + e^{i\pi N}) (2\hat{c}_j^{\dagger}\hat{c}_p^{\dagger} - \hat{c}_p \hat{c}_p^{\dagger} - \hat{c}_j^{\dagger}\hat{c}_j) + (1 - e^{i\pi N}) (2\hat{c}_j \hat{c}_p - \hat{c}_p^{\dagger}\hat{c}_j^{\dagger} - \hat{c}_j^{\dagger}\hat{c}_p^{\dagger}) \quad (6.27)$$

because

$$|w_j P_\alpha\rangle = (\hat{c}_j^{\dagger} + \hat{c}_p) |P_\alpha\rangle \ , \quad (6.28)$$

$$(-1)^{|\alpha|} |w_j P_\alpha\rangle = (\hat{c}_j^{\dagger} - \hat{c}_p) |P_\alpha\rangle \ , \quad (6.29)$$

$$(-1)^{|\alpha|} |P_\alpha\rangle = e^{i\pi N} |P_\alpha\rangle = \hat{P} |P_\alpha\rangle \ , \quad (6.30)$$

and the product of two operators $\hat{c}_j^{\dagger}\hat{c}_j$, $\hat{c}_j\hat{c}_p$ or $\hat{c}_j^{\dagger}\hat{c}_p^{\dagger}$ commutes with the parity operator $\hat{P}$.

In the further course of this thesis, only operators with an even number of Majorana fermions ($w_j$-operators) are considered and therefore only the positive parity subspace $\mathcal{K}^+$ spanned by the canonical basis vectors $|P_\alpha\rangle$ with even $|\alpha|$ is of importance.

The dissipative part of the Liouvillian restricted to the positive parity subspace is given by equation (6.22) with $\hat{L}_{jp}$ characterised by equation (6.27) and with $\exp(i\pi N) \to 1$ as $|\alpha| = 0, 2, 4, ..., $

$$\hat{L}_{\mu^+} = -2 (\hat{c}^{\dagger})^T (M + M^T) \hat{c} + 2 (\hat{c}^{\dagger})^T (M - M^T) \hat{c}^\dagger \ , \quad (6.31)$$

where the Lindblad operators are characterised by the components of the Hermitian matrix $M$,

$$M_{jp} = \sum_{\mu} t_{\mu,j} l_{\mu,p}^* \ . \quad (6.32)$$

The total Liouvillian restricted to $\mathcal{K}^+$ is given by

$$\hat{L}_+ = -2 (\hat{c}^{\dagger})^T (2iH + M + M^T) \hat{c} + 2 (\hat{c}^{\dagger})^T (M - M^T) \hat{c}^\dagger \ . \quad (6.33)$$

This representation allows for a transformation to a Majorana basis in operator space, in which the Liouvillian can easily be diagonalised and thus all eigenvectors can be constructed inclusive the zero-mode eigenvector, which corresponds to the non-equilibrium steady (NESS) state of the system. In order to do so, one defines a set of Majorana maps $\hat{a}_r = \hat{a}_r^{\dagger}$,

$$\hat{a}_{2j-1} = \frac{1}{\sqrt{2}} (\hat{c}_j + \hat{c}_j^{\dagger}) \ , \quad \hat{a}_{2j} = \frac{i}{\sqrt{2}} (\hat{c}_j - \hat{c}_j^{\dagger}) \ , \quad (6.34)$$
for \( r = 1, 2, ..., 4N \), which fulfill the anticommutation relation \( \{ \hat{a}_r, \hat{a}_s \} = \delta_{rs} \). In this basis the Liouvillian reads

\[
\hat{L}_+ = \hat{a}^T A \hat{a} + A_0 \mathbb{I}
\]  

(6.35)

with the identity map \( \mathbb{I} \) over \( K \), an antisymmetric complex \( 4N \times 4N \) matrix \( A \) whose entries can be specified explicitly,

\[
A_{2j-1,2p-1} = -2iH_{jp} - M_{jp} + M_{pj}, \\
A_{2j-1,2p} = -2H_{jp} + 2iM_{pj}, \\
A_{2j,2p-1} = 2H_{jp} - 2iM_{jp}, \\
A_{2j,2p} = -2iH_{jp} + M_{jp} - M_{pj},
\]  

(6.36)

and a coefficient \( A_0 \) fulfilling

\[
A_0 = 2 \text{tr}(M) = \sum_{j=1}^{2N} \beta_j.
\]  

(6.37)

The matrix \( A \) is called shape matrix of the Liouvillian. The eigenvalues \( \beta_r \) of an antisymmetric matrix of an even dimension come in pairs \( \pm \beta \). Thus, the eigenvectors \( \mathbf{v}_r \) and the eigenvalues of \( A \) can be labelled by

\[
A \mathbf{v}_{2j-1} = \beta_j \mathbf{v}_{2j-1}, \quad A \mathbf{v}_{2j} = -\beta_j \mathbf{v}_{2j}
\]  

(6.38)

with \( j = 1, 2, ..., 2N \) and an ordering of the eigenvalues \( \text{Re}(\beta_1) \leq \text{Re}(\beta_2) \leq ... \leq \text{Re}(\beta_{2N}) \leq 0 \). The eigenvalues \( \beta_j \) are called rapidities. In this formalism, the non-equilibrium steady state can be calculated efficiently as the eigenstate of \( \hat{L}_+ \) with eigenvalue 0,

\[
\hat{L}_+ |\text{NESS}\rangle = 0.
\]  

(6.39)

A further basis transformation to normal master mode creation and annihilation maps

\[
\hat{b}^\dagger_j = \mathbf{v}_{2j} \cdot \hat{a}, \quad \hat{b}_j = \mathbf{v}_{2j-1} \cdot \hat{a}
\]  

(6.40)

for \( j = 1, 2, ..., 2N \), which fulfill almost-canonical anticommutation relations

\[
\{ \hat{b}_j, \hat{b}_p \} = 0, \quad \{ \hat{b}^\dagger_j, \hat{b}^\dagger_p \} = 0, \quad \{ \hat{b}_j, \hat{b}^\dagger_p \} = \delta_{jp}.
\]  

(6.41)

where the creation map \( \hat{b}^\dagger_j \) is in general not the Hermitian adjoint of \( \hat{b}_j \). In this basis \( \hat{L}_+ \) can be written in a \( 2N \times 2N \) normal form

\[
\hat{L}_+ = -2 \sum_{j=1}^{2N} \beta_j \hat{b}^\dagger_j \hat{b}_j,
\]  

(6.42)
6. Lindblad description of open lattice systems

where $\hat{b}^\dagger_j \hat{b}_j$ is the occupation operator of the normal master mode $j$. One can interpret the non-equilibrium steady state $|\text{NESS}\rangle$ and its biorthonormal partner $\langle 1 |$ as right and left hand vacuum of the normal master mode maps

$$\langle 1 | \hat{b}_j = 0 , \quad \hat{b}_j |\text{NESS}\rangle = 0 . \quad (6.43)$$

One identifies again a Fock-space-like structure, which allows for the writing all biorthonormal left and right eigenstates of $\hat{L}_+ (\langle \Theta^L_L |)$ and $|\Theta^R_R\rangle$, by generating modes out of the left and right hand vacuum

$$\langle \Theta^L_L | = \langle 1 | \hat{b}^{\nu_1 \nu_2} \hat{b}^{\nu_3 \nu_4} \cdots \hat{b}^{\nu_{2n}}_1 , \quad |\Theta^R_R\rangle = \hat{b}^{\nu_1 \nu_2} \hat{b}^{\nu_3 \nu_4} \cdots \hat{b}^{\nu_{2n}}_2 |\text{NESS}\rangle \quad (6.44)$$

with normal master mode occupation numbers $\nu_j \in \{0,1\}$ and $\nu = (\nu_1, \nu_2, \ldots, \nu_{2n})$. The left and right eigenvalue equation reads

$$\langle \Theta^L_L | \hat{L}_+ = \lambda_\nu \langle \Theta^L_L | , \quad \hat{L}_+ |\Theta^R_R\rangle = \lambda_\nu |\Theta^R_R\rangle \quad (6.45)$$

with eigenvalues

$$\lambda_\nu = -2 \sum_{j=1}^{2N} \beta_j \nu_j . \quad (6.46)$$

The non-equilibrium steady state is unique only if the rapidities fulfil $\beta_j \neq 0 \forall j$, because otherwise a vector $\nu$ with $|\nu| \neq 0$ would exist for which $\lambda_\nu = 0$, and the steady state characterised by equation (6.39) would not be unique.

If the lattice possesses a translational symmetry, one can apply a Fourier transform to obtain a momentum space representation by following [15],

$$\hat{a}_{k,\lambda} = \frac{1}{\sqrt{N}} \sum_{m=1}^N \hat{a}_{m,\lambda} e^{i km} , \quad (6.47)$$

where $\hat{a}_{m,\lambda} = \hat{a}_{4m-\lambda}, \lambda = 1, 2, 3, 4$ and $m$ runs over all possible sites of the physical lattice. If one uses periodically boundary conditions at the edges of a unit cell of the lattice with $L$ sites to describe the bulk and expresses the shape matrix $A$ in the momentum space representation, equation (6.35) can be rewritten,

$$\hat{L}_+ - A_0 \mathbb{I} = \sum_{k=-\pi}^{\pi} \hat{a}_k^T \hat{L}_+(k) \hat{a}_k , \quad (6.48)$$

where $\hat{a}_k$ is a vector with $4L$ components and the antisymmetric $4L \times 4L$ matrix $\hat{L}_+(k)$ is to be seen in analogy to a energy shifted Bloch Hamiltonian and therefore is named Bloch Liouvillian. The antisymmetry of $\hat{L}_+$ originates from the antisymmetry of the shape matrix $A$ in equation (6.35), which transfers onto the Bloch Liouvillian. An exemplary calculation of the Bloch Liouvillian of an exemplary system can be found in appendix C.
6.2.1. Band theory of the Bloch Liouvillian

In analogy to the Hamiltonian band theory, the complex eigenvalues of a $4L \times 4L$ Bloch Liouvillian, which describes a chain of unit cells consisting of $L$ lattice sites form $2L$ bands of twofold degenerate eigenvalues. The eigenvalues of $\mathcal{L}_+$ come in pairs of $\pm E$ because of the antisymmetry $\mathcal{L}_+$. In addition, if $E$ is an eigenvalue, also the eigenvalue $E^*$ is found, i.e. out of eight eigenvalues ($E$, $-E$, $E^*$, and $-E^*$, where each of them is twofold degenerate) only one is really independent. The degeneration causes the bands to be actually gapless, what contradicts a direct analogy to the band theory of Bloch Hamiltonians. Such an analogy can be drawn by considering a degenerate band as a unity. The degenerate bands are gapped or may touch each other similarly to the bands of Bloch Hamiltonians. With regard to this interpretation, the degenerate subspaces of the basis of the Bloch Liouvillian have to be biorthonormalised. This allows for the evaluation of equation (3.17) using the left and right eigenstates of the Bloch Liouvillian in the scope this heuristic generalisation of the Hamiltonian band theory onto dissipative systems in the framework of third quantisation. If one extends the algorithm presented in chapter 4 such that the degenerate basis states are chosen to be biorthonormal and smooth, the numerical computation of the dissipative Zak phase similar to the complex Zak phase for the eigenstates of the Bloch Liouvillian becomes possible. The results of such computations are discussed in the following section.

6.3. Dissipative extensions of the SSH model

In this section, the algorithm introduced in chapter 4 is applied on the Bloch Liouvillian of the SSH model embedded in different baths to compute the dissipative Zak phase numerically. The Lindblad operators are chosen to describe single-particle gain (g) and loss (l),

$$L_{gm} = \sqrt{\Gamma} c_m^\dagger, \quad L_{lm} = \sqrt{\Gamma} c_m.$$

(6.49)

Starting from the Hamiltonian of the SSH model,

$$H_{SSH} = c^\dagger \begin{pmatrix} 0 & t_- & 0 & \cdots & t_+ \\ t_- & 0 & t_+ & \cdots & \vdots \\ 0 & t_+ & \cdots & t_- & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ t_+ & \cdots & t_- \end{pmatrix} c,$$

(6.50)

with periodic boundary conditions, one applies different periodic configurations of Lindblad operators in analogy to the complex potentials investigated in chapter 5 and calculates the corresponding Bloch Liouvlillians and the dissipative Zak phases of its eigenvalue.
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Figure 6.1.: Illustration of the dissipative SSH model with a bath causing alternating gain and loss. The $4 \times 4$ matrices $G$ describe single-particle gain ($g$) and loss ($l$) in the third quantisation formalism. In this figure the parameter $\Gamma$ is absorbed in the matrices $G$. The $4 \times 4$ matrices $T$ describe next neighbour hopping.

bands. Further the steady state is investigated with respect to its topology in systems with periodic boundary conditions and the occurrence of edge features in finite versions of the models. Therefore one uses an heuristic analogy between the steady state and the ground state in systems characterised by a Bloch Hamiltonian.

6.3.1. Bath with alternating gain and loss

The Lindblad operators $L_\mu$ (cf. equation (6.13)), which describe alternating gain and loss are characterised by

$$l_{\mu,j} = \begin{cases} \sqrt{\frac{\Gamma}{2}}, & j = 2m - 1 \quad \text{with } m = 1, 2, \ldots, N \\ \frac{1}{2} \sqrt{\Gamma}, & j = 2m \quad \text{with } m = 1, 3, \ldots, N - 1 \\ -\frac{1}{2} \sqrt{\Gamma}, & j = 2m \quad \text{with } m = 2, 4, \ldots, N \end{cases} \quad (6.51)$$

With these Lindblad operators applied to the SSH model, one obtains a lattice with unit cells comprising two sites, which is described by a Bloch Liouvillian of the form (cf. equation (6.48))

$$\mathcal{L}_+ - A_0 = \frac{1}{2} \sum_{k=-\pi}^{\pi} \left( |k,A\rangle \langle k,B| \right)^T \left( \Gamma G_g \left( t_- + e^{ik} t_+ \right) T \left( t_- + e^{-ik} t_+ \right) \Gamma G_l \right) \left( |k,A\rangle \langle k,B| \right)_{(8\times8)} =: \mathcal{L}_+ \quad (6.52)$$

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Figure 6.2.: Dissipative Zak phase of the steady state and states of the Bloch Liouvillian of the SSH model with alternating gain and loss in dependence of the dimerisation parameter $\theta$ and the parameter of gain and loss $\Gamma$. The system parameters are $t = 1$ and $\Delta = 0.5$. The imaginary part of the phase is found to be zero and the dissipative Zak phases of all eight eigenstates of the Bloch Liouvillian from equation (6.52) are the same. A phase transition occurs for $\theta = \pi/2$, where the band gaps between the degenerate bands of the Bloch Liouvillian vanish at $k = \pm \pi$ (indicated by a red line).

with

$$G_g = \begin{pmatrix} 0 & i & -i & 1 \\ -i & 0 & 1 & i \\ i & -1 & 0 & i \\ -1 & -i & -i & 0 \end{pmatrix}_{(4 \times 4)}, \quad G_l = \begin{pmatrix} 0 & i & i & -1 \\ -i & 0 & -1 & -i \\ -i & 1 & 0 & i \\ 1 & i & -i & 0 \end{pmatrix}_{(4 \times 4)},$$

(6.53)

$$T = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}_{(4 \times 4)}$$

where the matrices $G_g$, $G_l$, $T$ and the Bloch Liouvillian $\hat{L}_+$ are explicitly derived in appendix C. The Bloch Liouvillian is considered in a $4 \times 4$ block structure, in which the form of $\hat{L}_+$ reminds of the Bloch Hamiltonian describing the $\mathcal{PT}$-symmetric SSH model with alternating gain and loss (cf. equation (5.5)). This analogy is illustrated in figure 6.1.

A numerical investigation of the Bloch Liouvillian reveals that all eight eigenstates have the same dissipative Zak phase $\gamma$, which is why only one of them is shown in figure 6.2. The imaginary part of the numerically computed dissipative Zak phase vanishes, i.e. $\text{Im}(\gamma) = 0$. For $\theta < \pi/2$ the system is in the topologically nontrivial phase as the
dissipative Zak phase is equal to $\pi$. The degenerate bands of the Bloch Liouvillian from equation (6.52) are shown in figure 6.3, which should be seen in analogy to figures 2.3 and 5.4. A phase transition occurs for $\theta = \pi/2$ independently of the gain and loss rate $\Gamma$. At these points the band gaps between the eigenvalues $E$ and $E^*$ as well as $-E$ and $-E^*$ vanish, as the eigenvalue bands of the Bloch Liouvillian touch each other at $k = \pm \pi$. This behaviour is again in full analogy to the Bloch Hamiltonian scenario, were one can find band gap closings between Bloch bands at topological phase transitions. For other values of $\theta$ the degenerate bands of the Bloch Liouvillian are gapped in the sense that the dimension of the degenerate subspace is equal to two for all values of $k$. Compared with the $\PT$-symmetric case (see figure 5.3), the dissipative Zak phases calculated from the Bloch Liouvillian and the real part of the complex Zak phases obtained from the eigenvectors of the Bloch Hamiltonian match perfectly in the $\PT$-unbroken regime of the effective theory. In contrast to the $\PT$-symmetric description of open lattice systems by $\PT$-symmetric potentials (a discussion can be found in chapter 5), the degenerate bands are gapless only for one value of $\theta$, and not for an interval in which the quantisation of the complex Zak phase is repealed (e.g. in figures 5.4 and 5.3). The steady states of a finite version of this dissipative lattice model give rise to the possible occurrence of edge states in the system. The expectation values of the occupation number operators of the steady states obtained as the eigenstate of the Liouvillian with the eigenvalue equal to zero [43] are shown in figure 6.4. They visually reproduce the maximal $\PT$-broken ground states of the $\PT$-symmetric Hamiltonian (i.e. the ground state that corresponds to the eigenvalue with the smallest real part and the maximal imaginary part) which are investigated in the previous chapter (see figure 5.5 (b) and (d)). This motivates the approach of topologically classifying the steady state by a sum of the dissipative Zak phases of “occupied” bands as the ground state is classified by the
6.3. Dissipative extensions of the SSH model

Figure 6.4.: Steady states of the dissipative SSH model with alternating gain and loss in the two different topological phases with system parameters \( t = 1, \Delta = 0.5 \) and \( \Gamma = 0.5 \). The latter corresponds to a value of \( \Gamma = 1 \) when compared to the results of the investigation of \( \mathcal{PT} \)-symmetric Hamiltonians because of the different convention used in the Lindblad master equation in [43]. In (a) for \( \theta = \pi/5 \) and in (b) \( \theta = 4\pi/5 \).

sum of the Zak phases of occupied Bloch Bands. In this context it seems to be adequate to neglect the degeneracy of the eigenvalue bands of \( \hat{L}_+ \).

It can be seen that the steady state of the open SSH model with alternating gain and loss shows the same characteristic edge features as a \( \mathcal{PT} \)-broken ground state of the non-Hermitian SSH model with a complex potential effectively describing alternating gain and loss in the topologically nontrivial phase with a dissipative Zak phase of \( \gamma = \pi \) (cf. figure 5.5). The sites coupled to a reservoir describing particle gain exhibit a bigger occupation number expectation value as those coupled to a reservoir describing particle loss. This is also true for the steady state in the topologically trivial phase with \( \gamma = 0 \), which is shown in (b). The existence of edge states in the phase with \( \gamma = \pi \) and their absence in the phase characterised by \( \gamma = 0 \) as well as the vanishing of the eigenvalue band gap in the spectrum of the Bloch Liouvillian at \( k = \pm \pi \) at the phase transition support the designation of the phases as topological and the approach to characterise topologically phases in dissipative systems by the dissipative Zak phase.

The analogy between the maximal \( \mathcal{PT} \)-broken ground state (discussed in section 5.1) and the dynamical steady state seems to be appropriate because the maximal \( \mathcal{PT} \)-broken ground state dominates the unitary-like time evolution in the course of an effective description of open quantum systems. The probability to find the \( \mathcal{PT} \)-symmetric system in this state grows exponentially

\[
|\psi(t)\rangle = e^{-iE/\hbar t} |\psi(0)\rangle ,
\]

and it grows faster as the probability to find the system in another ground state because the imaginary part is maximal. Since the total particle number of fermionic lattice systems is restricted by the Pauli principle, it is reasonable that the system converges against the maximal \( \mathcal{PT} \)-broken ground state after some time, as a steady state in a real dynamical description. Thus, an open quantum system effectively described in the framework of non-Hermitian quantum mechanics is able to reproduce basic properties of a system described by Lindblad master equations. The question concerning the
6. Lindblad description of open lattice systems

Figure 6.5.: Illustration of the dissipative SSH model with a bath causing gain and loss at the edges of the unit cells with $L$ lattice sites in analogy to figure 6.1. Open and unfilled circles mark sites which are not coupled to the reservoir.

topological properties of the system can be clarified by investigating the analogous $\mathcal{P}\mathcal{T}$-symmetric model in the $\mathcal{P}\mathcal{T}$-unbroken parameter regime. This statement is supported by the investigation of another bath describing one-particle gain and loss at the edges of the lattice in the next part of this section.

6.3.2. Gain and loss at single sites at the borders of a unit cell

Starting point of the analysis is again the Hamiltonian of the SSH model (cf. equation (6.50)). In the following the SSH model is embedded into a reservoir with single-particle gain and loss at the edges of the unit cells with $L$ lattice sites. A sketch of the system can be found in figure 6.5. The Lindblad operators $L_\mu$ which characterise the reservoir are again given by equation (6.13), now with the coefficients

$$l_{\mu,j} = \begin{cases} \frac{\sqrt{\Gamma}}{2}, & j = 2m - 1 \quad \text{with } m = 1, N \\ \frac{i\sqrt{\Gamma}}{2}, & j = 2m \quad \text{with } m = 1 \\ -\frac{i\sqrt{\Gamma}}{2}, & j = 2m \quad \text{with } m = N \\ 0, & \text{elsewise} \end{cases}$$

(6.55)

The calculation shown in appendix C for alternating gain and loss can be analogously performed for this system with periodic boundary conditions resulting in a Bloch Liouvillian of the form

$$\mathcal{L}^+= \frac{1}{2} \begin{pmatrix} \Gamma G_g & t_- T & 0 & t_+ e^{ikT} \\ t_- T & 0 & t_+ T & \cdots \\ 0 & t_+ T & \cdots \\ t_+ e^{-ikT} & 0 & t_- T & \Gamma G_l \end{pmatrix}_{(4L \times 4L)}$$

(6.56)

with the $4 \times 4$ matrices $G_g, G_l, T$ given by equation (6.53), and the matrix 0 in which all components are equal to zero. Again the Bloch Liouvillian in the $4 \times 4$ block structure
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reminds of the form of the Bloch Hamiltonian of the analogous $\mathcal{PT}$-symmetric system which is given in equation (5.21).

The dissipative Zak phases resulting from a numerical integration of equation (3.17) using the 40 gauge smoothed and biorthonormalised eigenvector pairs of this Bloch Liouvillian are shown in figure 6.6. Each phase is obtained four times as the bands $E$ and $-E$ have the same dissipative Zak phase and each of them is twofold degenerate yielding a dissipative Zak phase twice. Additionally, the phases $\gamma_4$ and $\gamma_5$ are equal, which means that eight eigenvectors result in this dissipative Zak phase. On first sight, one can see that all phases are equal to zero for $\theta \to \pi$ and equal to $\pi$ for $\theta \to 0$ for some values of $\Gamma$, and therefore expects the topology of the system to change somewhere in between. The corresponding eigenvalue bands are shown in figure 6.7 for different values of $\theta$ and a fixed $\Gamma$. Different band gap closings can occur (meaning the simultaneous vanishing of the real and the imaginary part of the band gap and a local degeneration of the already
6. Lindblad description of open lattice systems

Figure 6.7.: Complex eigenvalue band structure of the Bloch Liouvillian of the SSH model subject to a bath characterising gain and loss at the edges of the unit cells, which contain 10 sites. The Bloch Liouvillian is a $40 \times 40$ matrix with 40 eigenvalues. The system parameters are $t = 1$, $\Delta = 0.5$, $\Gamma = 0.6$, and the corresponding values of $\theta$ are given above the graphs. Because of the degeneracies one finds 10 different real (solid blue and solid highlighted lines, left hand axis) resp. imaginary parts (solid red and dashed highlighted lines, right hand axis) which form 20 twofold degenerate eigenvalue bands occurring in pairs of $\pm E$. The relevant bands are highlighted in a bright colour with a solid line for their real part and a dashed line for their imaginary part. Note the two different axis for the real resp. imaginary part. Two different kinds of gap closings can be found, one where only the real resp. the imaginary part of the band gap between two bands vanish and one where the real and imaginary part of the gap vanish simultaneously. A band gap closing of the first type is shown on the left for $\theta = 3\pi/32$, and a gap closing of the latter type is shown in the centre for $\theta = 27\pi/64$, where the bands close for $k = \pm \pi$. This scenario is comparable to the simpler example of a $8 \times 8$ Bloch Liovillian (cf. figure 6.3 for $\theta = \pi/2$). On the right hand side the band structure is shown for $\theta = \pi$, where all dissipative Zak phases are found to be zero (cf. figure 6.6). The bands are found to be gapped.

degenerate bands). Two different types of gap closings are depicted in the first two graphs of figure 6.7. A vanishing of the band gap between a band $E$ and $E'$ is denoted in the following by $(E, E')$. On the left hand site a gap closing is shown, in which eight bands are involved. If one designates the yellow band with $E_{\text{yellow}}$ and the grey band with $E'_{\text{grey}}$, one can find the gap closings $(E_{\text{yellow}}, E'_{\text{grey}})$, $(-E_{\text{black}}, -E'_{\text{purple}})$, $(E^*_{\text{green}}, E'^*_{\text{brown}})$, and $(-E^*_{\text{pink}}, -E'^*_{\text{orange}})$, where the colours refer to the highlighted bands in figure 6.7. After a gap closing of this type the bands reopen and some parts of the eigenvalue branches are interchanged to allow for the identification of smooth eigenvalue bands.
6.3. Dissipative extensions of the SSH model

A second type of band gap closing occurs, in which only the four bands \( E, -E, E^*, -E^* \) participate, as the band gap of the imaginary parts of the bands vanish at \( k = \pm \pi \). This is illustrated in the centre of figure 6.7, where one can find the gap closings \( (E_{\text{yellow}}, E_{\text{green}}^*) \) and \( (-E_{\text{black}}, -E_{\text{pink}}^*) \), again the colours refer to the highlighted bands in figure 6.7. The remaining band gaps between \( \pm E \) and \( \pm E^* \) are real valued. The value of \( \theta \) at which these closings can be found vary with \( \Gamma \), and the dissipative Zak phase of the bands may change at all gap closings of these two types.

As mentioned before it seems to be appropriate to classify the steady state by the sum over the dissipative Zak phases of “occupied” bands of the Bloch Liouvillian, without taking into account the degeneracy of the band structure. This is illustrated in figure 6.8. In this course one counts the multiplicity of nontrivial dissipative Zak phases at each point of the parameter plane (spanned by \( \theta \) and \( \Gamma \)) and obtains a topologically nontrivial phase for odd and a trivial phase for even multiplicities of \( \pi \). The result of such an analysis is the phase diagram shown in figure 6.9. One finds a topologically nontrivial phase \( (\gamma = \pi \mod 2\pi) \) on the left hand side of the red line, which marks the points, for which the total band gap (real and imaginary part) vanishes (gap closing of the type, which shown in the center of figure 6.7).

Compared with the \( \mathcal{PT} \)-symmetric case (see figure 5.12), the dissipative Zak phase characterising the steady state (cf. figure 6.9) and the real part of the complex Zak phases obtained from the eigenvectors of the Bloch Hamiltonian (in case of unbroken
Figure 6.9.: Phases of the Liouvillian of the SSH model with alternating gain and loss in dependence of the dimerisation parameter $\theta$ and the parameter of gain and loss $\Gamma$. The system parameters are $t = 1$ and $\Delta = 1$. The gap closings $(E, E^*)$ and $(-E, -E^*)$ (gap closings of the type shown in the centre of figure 6.7) can be found at the red line.

Remarks

The heuristic generalisation of the Hamiltonian band theory onto open quantum systems described in the framework of third quantisation allows for the calculation of a Zak phase analogue, the dissipative Zak phase $\gamma$. This generalisation is in complete analogy to the Bloch Hamiltonian scenario. One finds topologically classifiable eigenvalue bands, which touch at a topological phase transition, and a steady state, that seems to be characterised by the sum of the dissipative Zak phases of each “occupied” band, as the ground state in the Bloch Hamiltonian scenario. Further one can find an astonishing
6.3. Dissipative extensions of the SSH model

Figure 6.10.: Steady states of the dissipative SSH model with alternating gain and loss in the two different topological phases with system parameters $t = 1$, $\Delta = 0.5$ and $\Gamma = 0.5$. The latter value corresponds to $\Gamma = 1$ when compared to the results of the investigation of $\mathcal{PT}$-symmetric Hamiltonians because of the different convention of the Lindblad master equation in [43]. In (a) for $\theta = \pi/5$ and in (b) for $\theta = 4\pi/5$.

correspondence between the dissipative Zak phase and the real part of the complex Zak phase of analogous open quantum systems in an effective $\mathcal{PT}$-symmetric description in the $\mathcal{PT}$-unbroken parameter regime. The detection of topologically nontrivial phases is substantiated as in this phase the steady states of finite versions of the system show characteristic edge features. Further, an analogy between the steady states and the maximal $\mathcal{PT}$-broken ground states respectively an excited maximal $\mathcal{PT}$-broken state with a significantly larger imaginary part of a comparable $\mathcal{PT}$-symmetric lattice can be found (cf. section 5) as the occupation number operator expectation values of the corresponding states reproduce each other. Thus, some characteristic features of a dissipative lattice system described in the framework of Lindblad master equations can be obtained from an effective non-Hermitian $\mathcal{PT}$-symmetric theory. It can be seen that the effective $\mathcal{PT}$-symmetric description of open lattice systems is able to reproduce basic properties of the dissipative system described by Lindblad master equations. The classification of topological phases in one-dimensional $\mathcal{PT}$-symmetric lattice systems by the real part of the complex Zak phase and the accordance of the complex and the dissipative Zak phase, as well as the accordance of maximal $\mathcal{PT}$-broken and steady states are signs for the validity of the approach using an effective $\mathcal{PT}$-symmetric theory for the description of open quantum systems. Basic questions concerning the topology of the dissipative system can be clarified by investigating an analogous $\mathcal{PT}$-symmetric model.

The steady states found in the dissipative versions of the SSH model indicate a possible application of dissipation in the experimental investigation of one-dimensional lattice systems. It should be possible to prepare a system in a state that shows edge features by coupling the edges of a dimerised lattice to a reservoir that causes particle gain on one edge of the lattice and particle loss on the other or alternating gain and loss. The state of the system relaxes exponentially to the steady state [43]. In case of a bath with gain and loss on the edges of the lattice, the system will be prepared in a state showing edge features independently of the dimerisation of the lattice. In case of the edges being strongly coupled to the neighbouring sites, it is possible to attribute these sites to the
reservoir, and one finds a state of the form shown in figure 6.10 on the right hand side, which matches up with a steady state of the type shown on the left hand side in a system of the same dimerisation, where the sites at the edges have been removed. Thus, for the detection of edge states in dissipative systems the exact dimerisation of a lattice is not crucial, as long alternating hopping amplitudes are realised.
7. Summary and Conclusion

Recently, a large interest in lattice systems subject to gain and loss with topologically nontrivial phases has arisen \cite{14-16, 20, 31-36, 39}. Most studies were performed in the case of balanced gain and loss often described with \(\mathcal{PT}\)-symmetric complex potentials. However, in large parts of literature the investigation of complex Zak phases (or more general Berry phases) of \(\mathcal{PT}\)-symmetric lattice systems is restricted to very simple systems, which allow for an easy Fourier transformation and an analytical treatment of the Bloch Hamiltonian. These types of studies will remain unable to obtain results for the complex Zak phase of more complicated systems, whose investigation is nevertheless desirable. As an answer to this problem, a reliable and robust tool allowing for the study of such systems was proposed in this thesis.

Therefore a numerical approach to this problem was chosen, which allows for the computation of complex Berry phases of various systems. Using this approach, dissipative extensions of the SSH model and the Kitaev chain were investigated. In the first part of this thesis, an effective description of dissipative systems by non-Hermitian \(\mathcal{PT}\)-symmetric complex potentials was used. Diverse approaches of defining topological invariants of such systems are present in literature, of which some are at least questionable. Thus, the topological characterisation of such systems is subject of current research \cite{18, 20, 24, 46}. In this thesis it was shown that the complex Berry phase is quantised (cf. section 3.2.1) when the \(\mathcal{PT}\) symmetry is unbroken and can be used as a topological index which characterises the topology of the dispersion relation of the corresponding Bloch Hamiltonian. Hence, a generalisation of the topological band theory to dissipative systems effectively described by \(\mathcal{PT}\)-symmetric Bloch Hamiltonians is straightforward \cite{41} and part of the discussion.

For a subsequent investigation of such systems, a numerical method was introduced in chapter 4, which is able to determine a gauge-smoothed biorthogonal basis of a \(\mathcal{PT}\)-symmetric Hamiltonian. This allows for the numerical calculation of the corresponding Berry connection, which is integrated along the system’s Brillouin zone to obtain numerical results of the complex Zak phase. This method was compared to already known analytical calculations for the SSH model with alternating gain and loss, and was found to perfectly reproduce the analytical results. Thus, the numerical method provides the basis for the identification of topological phases (indicated by a nontrivial complex Zak phase) in spatially periodic \(\mathcal{PT}\)-symmetric lattice systems. In the further course of chapter 5 the algorithm was applied to more complicated \(\mathcal{PT}\)-symmetric extensions of the SSH model, of which Zak phases cannot be accessed analytically. The identification of topologically nontrivial phases in these systems is supported by the investigation of
the ground states of finite versions of the corresponding models. Further $\mathcal{PT}$-symmetric extensions of the Kitaev chain are investigated. For those systems no real eigenvalue spectrum was obtained, but the results were found to be in good accordance with other studies on the same systems [19, 20, 63].

A further open question was the validity of the effective non-Hermitian description of dissipative effects, which was used in the previously discussion. Another approach to dissipative systems, which has also been used to study questions of topological order in dissipative systems [15], is the description of dissipation using Lindblad master equations. However, the relation of both approaches was never intensively studied. Thus, in the last part of this thesis (see chapter 6) the results of the study of $\mathcal{PT}$-symmetric lattice systems were compared to dissipative extensions of the SSH model in the framework of Lindblad master equations using the method of third quantisation.

By means of the identification of a Bloch Hamiltonian-like structure in the Liouvillian, a heuristic analogy to the topological band theory becomes possible. In doing so, a Bloch Hamiltonian analogue is defined (the Bloch Liouvillian), of which the eigenvalue bands can be characterised by a Zak phase analogue, which is called dissipative Zak phase in the scope of this thesis. A relation between the Bloch Liouvillian and the steady state was derived, which allows for the topological classification of steady states in the framework of Lindblad master equations. The generalisation of the topological band theory on Liouvillian systems was found in complete analogy to the Bloch Hamiltonian scenario.

The dissipative Zak phases of the energy bands and the steady states were investigated by applying the numerical method of chapter 4. In the parameter regimes in which the dissipative Zak phase is nontrivial, steady states were found, which possess characteristic edge features. This substantiates the approach of classifying topological phases in open quantum systems by the dissipative Zak phase. These steady states reproduce the occupation number operator expectation values of $\mathcal{PT}$-broken ground (and excited) states found in analogous $\mathcal{PT}$-symmetric systems. Further, the dissipative Zak phase is in perfect agreement with the results for the complex Zak phase in the accessible ($\mathcal{PT}$-unbroken) parameter regions. This correspondences between the effective non-Hermitian theory and the description via Lindblad master equations shows that basic insights to the topology of open quantum systems can be obtained from an effective $\mathcal{PT}$-symmetric model for the implementation of gain and loss.

Even though important questions in the relation of the topological classification and dissipative effects could be answered in the scope of this thesis, some points are still open. In particular, the definition of topological states as locally indistinguishable steady states of a gapped quantum many-body Liouvillian with a dissipative gap and a purity gap, which can be found in literature [15], motivates the question, weather one could extend the concept of the generalized winding number of interacting systems to the steady state of dissipative systems, and if the description of the topological phase transition using a dissipative gap and a purity gap reproduce the behaviour of the gap closing of the eigenvalue bands of the Bloch Liouvillian. In addition, one could verify the presumption
that the closing of the Bloch Liouvillian band gap is strongly related to the closing of
the dissipative and the purity gap of the steady state. Further, the basic concept of
the numerical method, which was developed in the course of this thesis, allows for the
investigation of various lattice systems, which are not part of the above discussion.
A. Fourier transform

To calculate the Bloch Hamiltonian of lattice systems exhibiting unit cells with more lattice sites one makes use of the spatially periodic structure of the lattice. To this end the Hamiltonian is written in a tensor product basis

\[ |\kappa_{n,i}\rangle = |n, i\rangle = |n\rangle \otimes |i\rangle \]

of one-particle states, where the first index labels the unit cells (external degree of freedom) and the second index is used to describe the internal structure of the unit cells with \( M \) lattice sites,

\[ H = \frac{N}{M} \sum_{n,m=1}^{N/M} \sum_{i,j=1}^{M} H_{\kappa_{n,i},\kappa_{m,j}} |n, i\rangle \langle m, j| , \tag{A.1} \]

with the abbreviation \( \kappa_{n,i} = (n-1) M + i \) and periodic boundary conditions.

The Fourier transform is obtained by expressing the external degrees of freedom in a plane wave basis,

\[ |n\rangle = \frac{1}{\sqrt{N/M}} \sum_{k=-\pi}^{\pi} e^{-i kn} |k\rangle , \tag{A.2} \]

where the sum runs over discrete values of \( k \) in steps of \( k = 2\pi/N \). If one inserts this relation into equation (A.1) and identifies the Kronecker symbol

\[ \delta_{kq} = \frac{1}{N/M} \sum_{n=1}^{N/M} e^{-in(k-q)} \tag{A.3} \]

one arrives at the expression

\[ H = \sum_{n,m=1}^{N/M} \sum_{i,j=1}^{M} \sum_{k,q=-\pi}^{\pi} H_{\kappa_{n,i},\kappa_{m,j}} |k, i\rangle \langle q, j| e^{-i(\kappa n-kq) + (m-n)q} \tag{A.4} \]

For lattice systems which allow for more than next neighbour hopping, transition elements between the sites \( l_{\text{max}} \) neighbouring unit cells occur. This means that all matrix elements \( H_{\kappa_{n,i},\kappa_{m,j}} \) with \( |m-n| > l_{\text{max}} \) vanish. In the following the abbreviation \( l = m-n \) is used. Because of the spatial periodicity of the lattice all matrix elements \( H_{\kappa_{n,i},\kappa_{m,j}} \) have to be independent of \( n \), this means \( H_{\kappa_{n,i},\kappa_{n+l,j}} = H_{\kappa_{1,i},\kappa_{1+l,j}} \) (roughly spoken all
A. Fourier transform

hopping processes that bring a particle out of a unit cell are reflected back). Thus one obtains from equation (A.4),

\[
H = \frac{N}{M} \sum_{n=1}^{l_{\text{max}}} \sum_{i,j=1}^{M} \sum_{l=-l_{\text{max}}}^{l_{\text{max}}} \frac{H_{\kappa_1,\kappa_1+l,j}}{N/M} |k,i\rangle \langle q,j| e^{-in(k-q)} e^{ilq}
\]

\[
= \sum_{l=-l_{\text{max}}}^{l_{\text{max}}} \sum_{i,j=1}^{M} \sum_{k,q=-\pi}^{\pi} H_{\kappa_1,\kappa_1+l,j} |k,i\rangle \langle q,j| e^{ilq} \delta_{kq}
\]

\[
= \sum_{l=-l_{\text{max}}}^{l_{\text{max}}} \sum_{i,j=1}^{M} \sum_{k=-\pi}^{\pi} H_{\kappa_1,\kappa_1+l,j} |k,i\rangle \langle k,j| e^{ilk}
\]

\[
= \sum_{k=-\pi}^{\pi} \left( |k,1\rangle, |k,2\rangle, \cdots, |k,M\rangle \right)
\]

\[
\text{e}^{ilk}
\]

\[
\left[
\begin{array}{cccc}
H_{\kappa_1,1,\kappa_1+l,1} & H_{\kappa_1,1,\kappa_1+l,2} & \cdots & H_{\kappa_1,1,\kappa_1+l,M} \\
H_{\kappa_1,2,\kappa_1+l,1} & H_{\kappa_1,2,\kappa_1+l,2} & \cdots & H_{\kappa_1,2,\kappa_1+l,M} \\
\vdots & \vdots & \ddots & \vdots \\
H_{\kappa_1,M,\kappa_1+l,1} & H_{\kappa_1,M,\kappa_1+l,2} & \cdots & H_{\kappa_1,M,\kappa_1+l,M}
\end{array}
\right]
\]

\[
\left[
\begin{array}{c}
|k,1\rangle \\
|k,2\rangle \\
\vdots \\
|k,M\rangle
\end{array}
\right]
\]

\[
= \mathcal{H} \text{ (Bloch Hamiltonian)}
\]
B. Zak phase and winding number

Here the Zak phases of the Hamiltonian $\mathcal{H}_\alpha = n_{\alpha,1}(k)\sigma_1 + n_{\alpha,2}(k)\sigma_2$ with eigenvalues $E_{\alpha,\pm}(k) = \pm \sqrt{n_{\alpha,1}(k)^2 + n_{\alpha,2}(k)^2} = \pm |n_\alpha(k)|$ and eigenstates

$|j_{\alpha,\pm}\rangle = \frac{1}{\sqrt{2}} \left( \frac{n_{\alpha,1} - in_{\alpha,2}}{\mp |n_\alpha|} \right)$

are calculated. In the following the index $\alpha$ is dropped for matters of clarity. The Zak phases are given by equation (2.13), which yield for the system considered here

$$
\gamma_\pm = i \oint_{BZ} \langle j_\pm | \partial_k | j_\pm \rangle \, dk
$$

$$
= \frac{i}{2} \oint_{BZ} \frac{n_1 - in_2}{\pm \sqrt{n_1^2 + n_2^2}} \partial_k \frac{n_1 - in_2}{\pm \sqrt{n_1^2 + n_2^2}} \, dk
$$

$$
= \frac{i}{2} \oint_{BZ} \frac{n_1 - in_2}{\sqrt{n_1^2 + n_2^2}} \times \left( \frac{\partial_k(n_1 - in_2)}{\sqrt{n_1^2 + n_2^2}} - \frac{(n_1 - in_2)^2(n_1\partial_k n_1 + n_2\partial_k n_2)}{\sqrt{n_1^2 + n_2^2}} \right) \, dk
$$

$$
= \frac{i}{2} \oint_{BZ} \frac{n_1 - in_2}{n_1^2 + n_2^2} \times \left( \partial_k n_1 - i\partial n_2 - \frac{n_2^2\partial_k n_1 + n_1 n_2\partial_k n_2 - in_1 n_2\partial_k n_1 - in_2^2\partial_k n_2}{n_1^2 + n_2^2} \right) \, dk
$$

$$
= \frac{i}{2} \oint_{BZ} \frac{n_1 - in_2}{n_1^2 + n_2^2} \frac{(n_2 - in_1)(n_2\partial_k n_1 - n_1\partial n_2)}{n_1^2 + n_2^2} \, dk
$$

$$
= \frac{1}{2} \oint_{BZ} \frac{n_1 \partial_k n_2 - n_2 \partial_k n_1}{n_1^2 + n_2^2} \, dk
$$

$$
= \pi \nu ,
$$

where in the last step the winding number was identified according to equation (2.44). Thus the Zak phases are related to the winding number of the vector $\alpha(k)$. 
C. Third quantisation of the SSH model

In the following the formalism of third quantisation is illustrated in the example of the SSH model. Starting point is the Hamiltonian of the SSH model with \( N \) lattice sites in the Nambu spinor space,

\[
H_{\text{SSH}} = c^\dagger \begin{pmatrix}
0 & t_- & 0 & \\
t_- & 0 & t_+ & 0 \\
0 & t_+ & 0 & t_- \\
0 & t_- & 0 & & \cdots & 0 & t_- & \cdots & \cdots & 0 & t_- & 0 \\
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_2 \\
\vdots \\
c_N
\end{pmatrix},
\] (C.1)

where here and in the following the subscript of the matrix gives the dimension of the matrix and \( c = (c_1, c_2, \ldots, c_m, \ldots, c_N)^T \). The transformation to the Majorana basis \( w_j = w_j^\dagger \) is achieved by a matrix multiplication reproducing the relations

\[
w_{2m-1} = c_m + c_m^\dagger , \quad w_{2m} = i(c_m - c_m^\dagger) ,
\]
\[
\implies c_m = \frac{1}{2}(w_{2m-1} - i w_{2m}) , \quad c_m^\dagger = \frac{1}{2}(w_{2m-1} + i w_{2m}) .
\] (C.2)

The transformation of \( \mathbf{w} = (w_1, w_2, \ldots, w_j, \ldots, w_{2N})^T \) to \( \mathbf{c} \) is given by

\[
\mathbf{c} = \frac{1}{2} \begin{pmatrix}
1 & -i & 0 & 0 & \\
0 & 0 & 1 & -i & \cdots & 0 & 0 & \\
0 & 0 & 0 & & \cdots & 0 & 0 & \\
1 & -i & & & \cdots & & & \\
\end{pmatrix}
\begin{pmatrix}
w_1 \\
w_2 \\
\vdots \\
w_{2N}
\end{pmatrix} ,
\] (C.3)
C. Third quantisation of the SSH model

whereas the transformation of the Hermitian adjoint vector $w^\dagger = (w_1, w_2, ..., w_j, ..., w_{2N})^T$ to $c^\dagger$ is given by

$$c^\dagger = \frac{1}{2} w^\dagger \begin{pmatrix} 1 & 0 & \cdots & 0 \\ i & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \\ 0 & 0 & \cdots & i \\ 0 & 0 & \cdots & 0 \\ \end{pmatrix}_{(2N \times N)} ,$$

such that the Hamiltonian of the SSH model is given by (cf. equation C.1)

$$H_{SSH} = \frac{1}{4} w^\dagger \begin{pmatrix} 1 & 0 & \cdots & 0 \\ i & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \\ 0 & 0 & \cdots & i \\ 0 & 0 & \cdots & 0 \\ \end{pmatrix}_{(2N \times 2N)} \begin{pmatrix} 0 & t_- & 0 & \cdots & 0 \\ t_- & 0 & t_+ & 0 & \cdots \\ 0 & t_+ & 0 & t_- & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & \cdots & 0 & t_- \\ 0 & 0 & \cdots & t_- & 0 \\ \end{pmatrix}_{(N \times N)}$$

$$= \frac{1}{4} w^\dagger \begin{pmatrix} 0 & 0 & t_- & -it_- & 0 & 0 \\ 0 & 0 & it_- & t_- & 0 & 0 \\ t_- & -it_- & 0 & 0 & t_+ & -it_+ \\ it_- & t_- & 0 & 0 & it_+ & t_+ \\ 0 & 0 & t_+ & -it_+ & 0 & 0 \\ 0 & 0 & it_+ & t_+ & 0 & 0 \\ \end{pmatrix}_{(2N \times 2N)} w .$$
This matrix has to be anti-symmetrised \( H_{SSH} \rightarrow 1/2(H_{SSH} - H_{SSH}^T) \) such that \( H_{SSH}^T = -H_{SSH} \).

\[
H_{SSH} = \frac{1}{4} \text{w}^\dagger \begin{pmatrix}
0 & 0 & 0 & -it_- & 0 & 0 \\
0 & 0 & it_- & 0 & 0 & 0 \\
0 & -it_- & 0 & 0 & 0 & -it_+ \\
it_- & 0 & 0 & 0 & it_+ & 0 \\
0 & 0 & 0 & -it_+ & 0 & 0 \\
0 & 0 & it_+ & 0 & 0 & 0
\end{pmatrix} \text{w} .
\] (C.6)

The matrix on the right side is \( H \) (cf. equation (6.19)). The next step is to set up the matrix \( M \) characterizing the Lindblad operators. Here Lindblad operators describing single particle gain (g) and loss (l) are used, which are alternatingly subject to the lattice sites of the SSH model,

\[
Lg_m = \sqrt{\Gamma} c_m^\dagger , \quad Ll_m = \sqrt{\Gamma} c_m ,
\] (C.7)

for \( m = 1, \ldots, N \) and the number of lattice sites \( N \). The vector \( l_{\mu} \) occurring in equation (6.13) is therefore given by

\[
L = \frac{1}{2} \begin{pmatrix}
1 & i & 0 & 0 & 0 \\
0 & 0 & -1 & i & 0 \\
0 & 0 & 1 & i & \ddots \\
0 & 0 & \ddots & \ddots & 0 \\
0 & 0 & 0 & \ddots & 1 & -i
\end{pmatrix} \text{w} ,
\] (C.8)

which leads to the coefficients

\[
l_{\mu,j} = \begin{cases}
\frac{\sqrt{\Gamma}}{2} , & j = 2m - 1 \quad \text{with } m = 1, 2, \ldots, N \\
\frac{i\sqrt{\Gamma}}{2} , & j = 2m \quad \text{with } m = 1, 3, \ldots, N - 1 \\
\frac{-i\sqrt{\Gamma}}{2} , & j = 2m \quad \text{with } m = 2, 4, \ldots, N
\end{cases} .
\] (C.9)

The components of the matrix \( M \) are given by equation (6.32) and the matrix \( M \) for alternating single-particle gain and loss reads

\[
M = \frac{\Gamma}{4} \begin{pmatrix}
1 & -i & 0 & 0 \\
i & 1 & 0 & 0 \\
0 & 0 & 1 & i & 0 \\
0 & 0 & -i & 1 & 0 \\
0 & 0 & 1 & -i & \ddots \\
0 & 0 & i & 1 & \ddots
\end{pmatrix} .
\] (C.10)
C. Third quantisation of the SSH model

Now the Liouvillian can be expressed through the matrices from equations (C.6) and (C.10) by using equation (6.19),

\[ \hat{\mathcal{L}}_+ = \hat{\mathcal{C}}^\dagger \begin{pmatrix} -\Gamma & 0 & 0 & -t_- & 0 & 0 \\ 0 & -\Gamma & t_- & 0 & 0 & 0 \\ 0 & -t_- & -\Gamma & 0 & 0 & -t_+ \\ t_- & 0 & 0 & -\Gamma & t_+ & 0 \\ 0 & 0 & 0 & -t_+ & -\Gamma & 0 \\ 0 & 0 & t_+ & 0 & 0 & -\Gamma \end{pmatrix} \hat{\mathcal{C}} \]

\[ (2N \times 2N) \]

(C.11)

\[ + \hat{\mathcal{C}}^\dagger \begin{pmatrix} 0 & -i\Gamma & 0 & 0 \\ i\Gamma & 0 & 0 & 0 \\ 0 & 0 & 0 & i\Gamma \\ 0 & 0 & -i\Gamma & 0 \\ 0 & 0 & 0 & -i\Gamma \end{pmatrix} \hat{\mathcal{C}}^\dagger \]

\[ (2N \times 2N) \]

The next step is to transform to the Hermitian Majorana maps defined in equation (6.34). The transformation of \( \hat{\mathbf{a}} = (\hat{a}_1, \hat{a}_2, ..., \hat{a}_r, ..., \hat{a}_{4N})^\dagger \) to \( \hat{\mathcal{C}} \) is given by

\[ \hat{\mathcal{C}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -i & 0 \\ 0 & 0 & 1 & -i \\ -i & 0 & 1 & i \\ 0 & -i & 0 & -i \end{pmatrix} \hat{\mathbf{a}}, \]

\[ (2N \times 4N) \]

(C.12)

and the transformation of \( \hat{\mathbf{a}}^\dagger = (w_1, w_2, ..., w_j, ..., w_{2N})^\dagger \) to \( \hat{\mathcal{C}}^\dagger \) is given by

\[ \hat{\mathcal{C}}^\dagger = \frac{1}{\sqrt{2}} \hat{\mathbf{a}}^\dagger \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & i & 1 \end{pmatrix} \]

\[ (4N \times 2N) \]

(C.13)
Using the equations (C.12) and (C.13) the Liouvillian $\mathcal{L}_{\text{SSH}}$ from equation (C.11) becomes

$$\hat{\mathcal{L}}_+ = \frac{1}{2} \hat{a}^\dagger \begin{pmatrix} \Gamma G_g & t_- T_0 & t_+ T_0 & 0 \\ t_- T_0 & \Gamma G_l & t_+ T_0 & 0 \\ 0 & t_+ T_0 & \Gamma G_g & t_- T_0 \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix} \hat{a}, \quad \text{(C.14)}$$

where the $4N \times 4N$ matrix is the matrix $A$ occurring in equation (6.35), which has to be chosen to be antisymmetric $A \rightarrow 1/2(A - A^T)$ such that $A^T = -A$. The matrices $G_g$ and $G_l$ result from Lindblad operators describing gain (g) respectively loss (l). For the matrices $G_g, G_l, T$ and $0$ one finds

$$G_g = \begin{pmatrix} 0 & i & -i & 1 \\ -i & 0 & 1 & i \\ i & -l & 0 & i \\ -1 & -i & -i & 0 \end{pmatrix}, \quad G_l = \begin{pmatrix} 0 & i & i & -1 \\ -i & 0 & -1 & -i \\ -i & 1 & 0 & i \\ 1 & i & -i & 0 \end{pmatrix}, \quad \text{(C.15)}$$

$$T = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad 0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad \text{(C.15)}$$

The Liouvillian from equation (C.14) can be rewritten by separating internal and external degrees of freedom such that the Fourier transform can be applied following the standard procedure (cf. appendix A),

$$\hat{\mathcal{L}}_+ = \frac{1}{2} \sum_{n=1}^{N/2} \left( t_- T_0 |n, A\rangle \langle n, B| + \text{h.c.} \right. \right.

$$+ t_+ T_0 |n, B\rangle \langle (n \text{ mod } N/2) + 1, A| + \text{h.c.} \right.

$$+ \Gamma G_g |n, A\rangle \langle n, A| + \Gamma G_l |n, B\rangle \langle n, B|, \quad \text{(C.16)}$$

where the Hermitian conjugate (h.c.) is to be interpreted line by line and

$$|n, A\rangle = \begin{pmatrix} \hat{a}_{4n-3} \\ \hat{a}_{4n-2} \\ \hat{a}_{4n-1} \\ \hat{a}_{4n} \end{pmatrix}, \quad |n, B\rangle = \begin{pmatrix} \hat{a}_{8n-3} \\ \hat{a}_{8n-2} \\ \hat{a}_{8n-1} \\ \hat{a}_{8n} \end{pmatrix} \quad \text{(C.17)}$$

with $n = 1, \ldots, N/2$ labelling the unit cells. Equation (C.16) can be interpreted as a tight-binding model with two different tunnelling amplitudes $t_-$ and $t_+$ and two different
C. Third quantisation of the SSH model

Figure C.1.: Illustration of the dissipative SSH model with a bath causing alternating gain and loss. The $4 \times 4$ matrices $G$ describe single-particle gain (g) and loss (l) in the third-quantisation formalism. In this figure the parameter $\Gamma$ is absorbed in the matrices $G$. The $4 \times 4$ matrices $T$ describe next-neighbour hopping.

lattice sites labelled with A and B, which differ by their “on-site potential” (see figure C.1). Again one expresses the external degrees of freedom in a plane wave basis

$$|n\rangle = \frac{1}{\sqrt{M}} \sum_{k=-\pi}^{\pi} e^{-ikn} |k\rangle$$  \hspace{1cm} (C.18)

and identifies the Kronecker symbol

$$\delta_{kq} = \frac{1}{M} \sum_{n=1}^{M} e^{-in(k-q)}.$$  \hspace{1cm} (C.19)

By inserting these relations to equation C.16 one finds

$$\hat{L}_+ = \frac{1}{2} \frac{1}{N/2} \sum_{n=1}^{N/2} \sum_{k,q=-\pi}^{\pi} \left( t_- T |k,A\rangle \langle q, B| e^{-in(k-q)} + h.c. \right.$$  

$$+ t_+ T |k, B\rangle \langle q, A| e^{-in(k-q)} e^{ik} + h.c. \right.$$  

$$+ \Gamma G_g |k,A\rangle \langle q, A| e^{-in(k-q)}$$  

$$+ \Gamma G_l |k,B\rangle \langle q, B| e^{-in(k-q)} \right)$$  

$$= \frac{1}{2} \sum_{k,q=-\pi}^{\pi} \left( t_- T |k,A\rangle \langle q, B| \delta_{kq} + h.c. \right.$$  

$$+ t_+ T |k, B\rangle \langle q, A| \delta_{kq} e^{ik} + h.c. \right.$$  

$$+ \Gamma G_g |k,A\rangle \langle q, A| \delta_{kq} + \Gamma G_l |k, B\rangle \langle q, B| \delta_{kq} \right)$$  

$$= \frac{1}{2} \sum_{k=-\pi}^{\pi} \left( t_- T |k,A\rangle \langle k, B| + t_+ T |k, B\rangle \langle k, A| e^{ik} + h.c. \right.$$  

$$+ \Gamma G_g |k,A\rangle \langle q, A| + \Gamma G_l |k, B\rangle \langle q, B| \right).$$  

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This can be rewritten in a Nambu basis-like matrix structure, where as the matrix occurring on the right hand side is here denoted as Bloch Liouvillian $G_g$,

$$\hat{\mathcal{L}}_+ = \frac{1}{2} \sum_{k=-\pi}^{\pi} \begin{pmatrix} \langle k, A \rangle \langle k, B \rangle \\ \langle k, B \rangle \langle k, A \rangle \end{pmatrix}^T \begin{pmatrix} \Gamma G_{G_g} & \Gamma G_1 \\ \Gamma G_1 & \Gamma \end{pmatrix} \begin{pmatrix} t_- + e^{i k t_+} \\ t_- - e^{-i k t_+} \end{pmatrix} \begin{pmatrix} \langle k, A \rangle \\ \langle k, B \rangle \end{pmatrix}.$$  

(C.21)  

\[\hat{\mathcal{L}}_+ =: \hat{\mathcal{L}}_+ (\text{Bloch Liouvillian})\]
D. Summary (in German)

In der vorliegenden Masterarbeit mit dem deutschen Titel „Charakterisierung und Untersuchung topologisch nichttrivialer Zustände in \( \mathcal{PT} \)-symmetrischen fermionischen Vielteilchensystemen“ wurde die von abgeschlossenen Systemen bekannte topologische Bandtheorie auf offene Systeme erweitert. Dadurch konnten offene Fragen, welche die Klassifizierung von topologischen Phasen in dissipativen Systemen betreffen, beantwortet werden. Dabei wurden dissipative Erweiterungen des eindimensionalen SSH-Modells untersucht. Im ersten Teil der Arbeit wurde die Berry-Phase behandelt (Kapitel 2) sowie in Kapitel 3 an eine bereits bekannte, effektive, nichthermitesche Theorie herangeführt, die \( \mathcal{PT} \)-symmetrische Hamilton-Operatoren zur Beschreibung von dissipativen Systemen (mittels komplexen \( \mathcal{PT} \)-symmetrischen Potentialen) verwendet. In der Literatur existieren verschiedene Herangehensweisen, die es ermöglichen, die Topologie solcher Systeme zu untersuchen. Im Rahmen dieser \( \mathcal{PT} \)-symmetrischen Theorie konnte in Kapitel 3 gezeigt werden, dass der Realteil der komplexen Berry-Phase im \( \mathcal{PT} \)-ungebrochenen Bereich des Hamilton-Operators quantisiert ist und die topologische Klassifizierung der zugehörenden Bandstruktur ermöglicht. Dieser Ansatz wird im weiteren Verlauf der Arbeit verfolgt und ausgebaut.

In der Literatur wurden bislang meist einfache \( \mathcal{PT} \)-symmetrische Beispiele, welche analytisch zugängliche Lösungen besitzen, hinsichtlich deren Topologie untersucht. Die Behandlung von Modellen, die kompliziertere Gewinn- und Verlusteffekte aufweisen, ist jedoch wünschenswert, da diese experimentell zugängliche, in der Natur vorkommende Systeme effektiv beschreiben. Um solche Modelle hinsichtlich der Topologie der Bandstrukturen untersuchen zu können, wurde in Kapitel 4 ein Algorithmus eingeführt, der die numerische Berechnung des komplexen Berry-Potentials in einer einheitlichen Eichung entlang geschlossener Kurven im Parameterraum ermöglicht, indem eine glatte Eichung der biorthogonalen Basiszustände eines \( \mathcal{PT} \)-symmetrische Hamilton-Operators aufgestellt wird. Das resultierende Berry-Potential erlaubt es, durch eine numerische Integration die korrespondierende komplexe Berry-Phase zu berechnen.

In Kapitel 5 wurde dieser Algorithmus verwendet, um die Bandstrukturen verschiedener, durch komplexe, \( \mathcal{PT} \) symmetrische-Potentiale erweiterte, dissipative Versionen des SSH-Modells zu untersuchen. Hierbei wurden periodische Randbedingungen verwendet, um unendlich lange Gitter zu simulieren. Dabei konnte für ein bereits in der Literatur bekanntes analytisch zugängliches Modell eine perfekte Übereinstimmung von numerischen und analytischen Ergebnissen gefunden werden. Zusätzlich zu der Klassifizierung der Bandstrukturen wurden die Vielteilchengrundzustände endlicher Versionen der Systeme mit Hilfe einer exakten Diagonalisierung untersucht. In topologisch nicht-
trivialen Phasen wiesen die Grundzustände Randeigenschaften auf, was die Kennzeichnung dieser als Randzustände erlaubt. Weiter können Zustände mit komplexen Energieeigenwerten gefunden werden, die einen gleichen (oder zumindest einen ähnlichen) Realteil aufweisen. Unter anderem konnten Zustände mit maximalem Imaginärteil (maximal $\mathcal{PT}$-gebrochene Zustände) gefunden werden, die das System in einer unitärtigen Zeitauslassung dominieren.


Offen blieben dabei einige Fragen, welche die Topologie des stationären Zustandes der dissipativen Systeme betreffen. Zum Beispiel stellt sich die Frage, ob die verallgemeinerte Windungszahl (Zak-Phase) für wechselwirkende Systeme mit Hilfe des stationären Zustandes auf dissipative Systeme im Rahmen einer Beschreibung durch Lindblad-Mastergleichungen erweitert werden kann. Weiter könnte der Zusammenhang zwischen dem Verschwinden der Bandlücke der Eigenwertbänder des Liouville-Operators in Bloch-Gestalt und dem Verschwinden der Reinheits- und der dissipativen Lücke untersucht werden, was in der Literatur für den topologischen Phasenübergang vorausgesagt wurde. Zusätzlich erlaubt die in Rahmen dieser Masterarbeit entwickelte numerische Methode die Untersuchung einer Vielzahl an Systemen, die nicht Teil der obigen Diskussion sind.

Insgesamt konnte gezeigt werden, dass die effektive $\mathcal{PT}$-symmetrische Beschreibung in der Lage ist, wichtige Eigenschaften offener Quantensysteme korrekt zu beschreiben, und dass grundlegende Eigenschaften der Topologie dissipativer Systeme aus dieser effektiven Theorie gewonnen werden können.
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Erklärung

Ich versichere,

- dass ich diese Masterarbeit selbständig verfasst habe,
- dass ich keine anderen als die angegebenen Quellen benutzt und alle wörtlich oder sinngemäß aus anderen Werken übernommenen Aussagen als solche gekennzeichnet habe,
- dass die eingereichte Arbeit weder vollständig noch in wesentlichen Teilen Gegenstand eines anderen Prüfungsverfahrens gewesen ist,
- und dass das elektronische Exemplar mit den anderen Exemplaren übereinstimmt.

Stuttgart, den 27. Oktober 2017

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