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Non-Bloch Band Theory of Non-Hermitian Systems

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Chapter 1 Introduction

1.1 Background

The conventional Bloch band theory in crystals is fundamental for describing electronic structure. By introducing the Bloch wave vector $\boldsymbol{k}$, energy bands calculated within a unit cell reproduce those of a large crystal with open boundaries. Here it is implicitly assumed that in the limit of a large system size, electronic states are almost equivalent between a system with open boundaries and one with periodic boundaries, represented by the Bloch wave function with real $\boldsymbol{k}$. This is because the electronic states extend over the system in both cases, implying that the effects of boundary conditions becomes negligible in the limit of a large system size.

Since the discovery of the quantum Hall effect, topological phases have been one of the most studied themes in condensed matter physics. In many previous studies, rich aspects of the topological phases have been theoretically investigated, and topological phenomena have been experimentally observed. For example, in crystals, as a manifestation of topological physics, there appears bulk-edge correspondence between a topological invariant defined in terms of the Bloch wave functions and existence of topological edge states localized at ends of the system. In fact, the bulk-edge correspondence is realized in some materials, and this result justifies the description of the Bloch band theory in topological systems. Recently, the notion of the topology has been extended from electronic systems to artificial systems, such as optical-lattice systems and metamaterials.

In recent years, interest in studies on non-Hermitian physics has been rapidly growing both in theories and in experiments. Historically, in a scattering problem, the resonant scattering in terms of a complex potential was the first study on the non-Hermitian physics [1]. After that, Ref. [2] proposed that Anderson localization, such as flux pinning in a superconductor, can be studied by using a non-Hermitian model. Recently, with the development of laser technology, non-Hermitian systems can be experimentally realized in various realistic systems, and studies on the non-Hermitian physics have been dramatically progressing. Such systems are described by a non-Hermitian Hamiltonian, and it is useful for studying non-equilibrium systems and open systems, which exchange energies and particles with external environment. Non-Hermitian systems emerge in various fields of classical physics and quantum physics. In classical systems, such as spring-mass systems, optical systems, and electric-circuit systems, gain and loss lead to non-Hermitian terms in eigenvalue equations. In particular, parity-time symmetry has been intensively studied to realize some phenomena unique to non-Hermitian systems, particularly in optical systems [3–5], as explained in detail in Chapter 2. Besides, topological laser has been also experimentally investigated [7, 8], and for example, it was proposed that a topological edge state can be amplified [6]. On the other hand, in quantum systems, open quantum systems, such as cold-atom systems, are one of the most useful platforms realizing non-Hermitian systems [9–11]. For example, Ref. [12] theoretically proposed the experimental realization of asymmetric hopping amplitude in a one-dimensional (1D) optical-lattice, where the system has the hopping amplitude to right different from that to left. Furthermore, a cold-atom system with Bose-Einstein condensation can be described by a Bogolibov-de Gennes (BdG) Hamiltonian, and it behaves as a non-Hermitian systems. Reference [13] experimentally confirmed that this non-Hermitian system exhibits dynamical instability. In theories, some previous works studied non-Hermitian phenomena caused by the dynamical instability in optical-lattice systems [14–18]. Besides, one of the origins of non-Hermiticity is many-body correlation effect, for example, in electronic systems [19].

Among many studies on non-Hermitian systems, one of the most intriguing topics is how non-Hermitian effects affect topological physics. Reference [20] first proposed that a topological invariant defined in a 1D non-Hermitian tight-binding model takes a fractional value, and localized edge states appear corresponding to the nonzero topological invariant. This previous work also mentioned the generalization of the bulk-edge correspondence in non-Hermitian systems. After this proposal, the bulk-edge correspondence in non-Hermitian systems has been much studied in theories. However it has been controversial in this field because many previous works have revealed the violation of the conventional bulk-edge correspondence in non-Hermitian systems. Hence, while the description of eigenstates in terms of real wave vector $\boldsymbol{k}$ is justified in Hermitian systems by the conventional Bloch band theory, it is not the case in non-Hermitian systems. With this background, pioneering previous research [21] proposed non-Hermitian skin effect. The non-Hermitian skin effect means that bulk eigenstates of non-Hermitian systems are localized at either end of an open chain. This phenomenon causes difference between energy eigenvalues in a system with open boundary conditions and those with periodic boundary conditions. Furthermore this previous work also mentioned that the eigenstates behave as "non-Bloch" wave, where the wave functions are well aproximated by Bloch-like waves with complex wave number. We will discuss these points in Chapter 2 and in Chapter 3.

Since then, the non-Hermitian skin effect has been one of the hottest topics in researches on non-Hermitian physics. In particular, many previous works have been focusing on topological structure of the non-Hermitian skin effect. After the proposal of a topological invariant, called energy winding number, defined in 1D non-Hermitian systems with a periodic boundary condition [12], Refs. [22] and [23] proposed a new type of the bulk-edge correspondence in non-Hermitian systems. Namely, when the energy winding number in a periodic chain takes nonzero values, bulk eigenstates are localized at edges of an open chain. Thus the correspondence between a non-Hermitian open chain and a non-Hermitian periodic chain was revealed. On the other hand, a lack of researches on a non-Hermitian open chain has been a long-standing issue. Although Ref. [21] showed the calculation of energy bands and Brillouin zone in 1D non-Hermitian systems in term of the conventional Bloch band theory, its method is applicable only to a very limited class of non-Hermitian systems, and it is needed to extend this method to general cases. Thus, due to the non-Hermitian skin effect, we should modify the Bloch band theory in non-Hermitian systems in order to discuss the bulk-edge correspondence and to study non-Hermitian physics.

Based on the idea of the non-Hermitian skin effect and the description of the non-Bloch wave, in this thesis, we construct a non-Bloch band theory of non-Hermitian crystalline systems with open boundary conditions. From our theory, in non-Hermitian systems, we can determine the Brillouin zone reproducing energy bands in a long open chain. Thus the non-Bloch band theory is fundamental for non-Hermitian physics, and therefore, this theory can reveal various aspects of non-Hermitian systems. Firstly, a byproduct of our theory is that one can prove the bulk-edge correspondence between a topological invariant defined in the bulk and existence of localized edge states in general non-Hermitian systems. In fact, we will demonstrate the bulk-edge correspondence in the non-Hermitian Su-Schrieffer-Heeger (SSH) model in Chapter 4. Secondly, we can find a new type of a gapless phase in non-Hermitian systems in terms of the non-Bloch band theory. We will show that this gapless phase is stabilized because of the modification of the Brillouin zone in Chapter 5. Thirdly, we can study non-Hermitian nature of a bosonic system described by a Bogoliubov-de Gennes (BdG) Hamiltonian. While some previous works studied non-Hermiticity in a finite system under open boundary conditions by numerical calculation, non-Hermitian physics in a bosonic BdG system in the thermodynamic limit has been unrevealed yet. Hence the non-Bloch band theory can clarify general non-Hermitian properties in such a system. In fact, in terms of this theory, we will show rich aspects of the non-Hermitian skin effect, i.e. infinitesimal instability and reentrant behavior, in Chapter 6.

1.2 Outline

This thesis is organized to establish the Bloch band theory in non-Hermitian systems and to study various properties of non-Hermitian systems as mentioned in Sec. 1.1. The organization of this thesis is the following.

In Chapter 2, first of all, we start with the review of topological physics in Hermitian systems. We introduce two kinds of topological insulators and explain how these insulating phases can be topologically classified. Furthermore, in the SSH model, we derive a $\mathbb{Z}$ topological invariant from a Q matrix and demonstrate the bulk-edge correspondence. Next we review non-Hermitian systems. We particularly focus on a parity-time symmetry, which is one of the most studied topics in non-Hermitian systems. Throughout the discussion, we give the notion of an exceptional point, and explain that such non-Hermitian degeneracy can appear not only in the parameter space but also in the momentum space. Finally we show the violation of the bulk-edge correspondence in the non-Hermitian SSH model, caused by the non-Hermitian skin effect.

In Chapter 3, in order to discuss the non-Hermitian skin effect, we compare the behaviors in non-Hermitian systems with open boundary conditions with those with periodic boundary conditions. In particular, we deeply analyze the difference between the energy eigenvalues and the behaviors of the eigenstates by using the simple model.

In Chapter 4, we establish a non-Bloch band theory in 1D tight-binding non-Hermitian systems. In an open chain, we show a way to determine the generalized Brillouin zone (GBZ) for the complex Bloch wave number $\beta = \mathrm{e}^{ik},\ k \in \mathbb{C}$. Then we see some aspects of the GBZ in some models. Furthermore, in the non-Hermitian SSH model, we demonstrate the bulk-edge correspondence between the topological invariant defined by the GBZ and the appearance of the topological edge states. We further comment on the existence of the gapless phase in the non-Hermitian SSH model in this chapter.

In Chapter 5, according to the discussion in Chapter 4, we investigate a gapless phase which appears in the non-Hermitian SSH model. Then we show that in 1D non-Hermitian systems with sublattice symmetry and time-reversal symmetry, a gapless phase with exceptional points is stabilized because of the unique features of the GBZ. Furthermore we also find that each energy band is divided into three regions depending on the symmetry of the eigenstates.

In Chapter 6, we construct the non-Bloch band theory in bosonic BdG systems. We show that one can calculate the energy eigenvalues and can study general non-Hermitian properties in such systems with open boundary conditions in the thermodynamic limit. Furthermore we investigate the bosonic Kitaev-Majorana chain by using this theory. As a result, we show rich aspects of the non-Hermitian skin effect, such as infinitesimal instability and reentrant behavior.

In Chapter 7, we summarize this thesis and comment on outlook of the non-Bloch band theory.

List of Publications and Preprints

List of publications

Original papers

1. Kazuki Yokomizo and Shuichi Murakami,
   "Topological semimetal phase with exceptional points in one-dimensional non-Hermitian systems,"
   Physical Review Research **2**, 043045 (2020).

2. Kazuki Yokomizo and Shuichi Murakami,
   "Non-Bloch Band Theory of Non-Hermitian Systems,"
   Physical Review Letter **123**, 066404 (2019).

3. Kazuki Yokomizo, Hiroaki Yamada, and Shuichi Murakami,
   "Nodal-line superlattices,"
   Journal of Physics: Condensed Matter **30**, 505301 (2018).

4. Kazuki Yokomizo and Shuichi Murakami,
   "Topological phases in a Weyl semimetal multilayer,"
   Physical Review B **95**, 155101 (2017).

Review article

1. Kazuki Yokomizo and Shuichi Murakami,
   "Non-Bloch band theory and bulk-edge correspondence in non-Hermitian systems,"
   Progress of Theoretical and Experimental Physics **2020** (2020).

List of preprints

1. Ryo Okugawa, Ryo Takahashi, and Kazuki Yokomizo,
   "Second-order non-Hermitian skin effect,"
   arXiv: 2008.03721.