PHYS379: Group Project – Topology in Tight-Binding Models Topic

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Introduction

In PHYS379, you should undertake an open-ended group project and submit a group report describing the project. The group project is worth twenty credits. Please see the document "PHYS379-group-project-notes.pdf" for details about organisation and assessment.

Open-ended project

Your task in the project is to model the topological properties of a tight-binding model. Precisely what you do is your choice - the project is open-ended. You will need to formulate a research question (or questions) that is more specific than simply "model the topological properties of a tight-binding model". What are you trying to discover? You should do some research in the library or on the internet to find out what the interesting questions are. It may be that you will not finalise the research question until the latter stages of the project, once you have found what is (or is not) interesting. Remember that this is group work - it will make sense to plan for parallel tasks in order to use your personnel effectively. For example, you might want parallel numerical and analytic investigations, investigations looking at different aspects of the same problem, or you might deliberately duplicate effort in order to check important results (in the "real" world, results should always be checked before publication, getting different people to work independently is the best way to do this). There are some ideas below, you can follow some or all of them, or you can follow your own ideas.

Getting started

The SSH model in real space

The Su-Schrieffer-Heeger (SSH) model [1] is a tight-binding model of a one-dimensional chain with staggered hopping. It was introduced as a model of polyacetylene (which has alternating single and double bonds). It's also the simplest model of a topological insulator. Here, I will briefly describe the model, but please look at Chapter 1 of Ref.[2] which describes the model in depth.

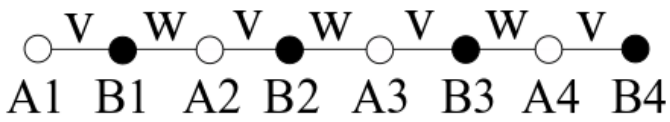

Figure 1 Schematic of the SSH chain with $N = 4$ unit cells with staggered hoppings v and w.

A schematic of the SSH model with $N = 4$ unit cells is shown in Fig.1. Nearest-nearest hoppings are either v or w: v is intracell and w is intercell. Generally $v \neq w$, so there are two atoms per repeating unit cell: they are denoted A and B. For $N = 4$, in a basis of A1, B1, A2, B2, A3, B3, A4, B4 (assuming one electronic orbital per atom), the tight-binding Hamiltonian is

$$H = \begin{pmatrix} 0 & v & 0 & 0 & 0 & 0 & 0 & 0 \\ v & 0 & w & 0 & 0 & 0 & 0 & 0 \\ 0 & w & 0 & v & 0 & 0 & 0 & 0 \\ 0 & 0 & v & 0 & w & 0 & 0 & 0 \\ 0 & 0 & 0 & w & 0 & v & 0 & 0 \\ 0 & 0 & 0 & 0 & v & 0 & w & 0 \\ 0 & 0 & 0 & 0 & 0 & w & 0 & v \\ 0 & 0 & 0 & 0 & 0 & 0 & v & 0 \end{pmatrix}$$

The main diagonal describes the on-site energy of each atom. Each atom can be assumed to be identical, so the on-site energy (which is the same for all) can be set equal to zero without loss of generality.

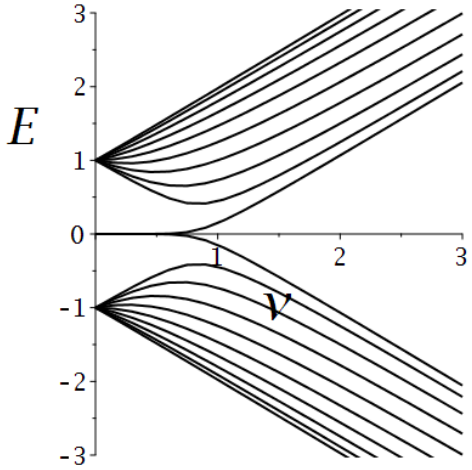

Figure 2 Plot of energies E as a function of intracell hopping v for fixed intercell hopping $w = 1$ for $N = 10$ unit cells. This is the same as Fig.1.4(a) in Ref.[2].

The eigenenergies E obtained by diagonalizing H are plotted in Fig.2 as a function of intracell hopping v for fixed intercell hopping $w = 1$ for $N = 10$ unit cells. This plot shows there are no states near $E = 0$ for $v > w$, but there are two states near $E = 0$ for $v < w$. It turns out that the two states near $E = 0$ for $v < w$ are localised on the edges of the system (see Fig.1.4 in Ref.[2]). It means the "bulk" of the system is an insulator, but there are "metallic" states at the edges.

The SSH model in k space

This can be related to a topological property of the Hamiltonian. For an infinite SSH chain with translational invariance, the Hamiltonian can be written in wave vector k space, simply as a 2×2 matrix in a basis of wave functions on A and B sites [2]:

$$H = \begin{pmatrix} 0 & v + we^{-ik} \\ v + we^{ik} & 0 \end{pmatrix}$$

It's possible to define a "winding number" for this Hamiltonian [2], and it takes the value of 0 for the trivial phase $v > w$ (when there are no edge states), but the value of 1 for the nontrivial topological phase $v < w$ (when there are edge states). This is an example of a topological invariant. In two-dimensional systems, the appropriate topological invariant is usually the Chern number.

Chiral symmetry

The SSH model has chiral symmetry (for a technical reason this is important for one-dimensional topological insulators). It basically means that terms in H only contact As with Bs, never As with As or Bs with Bs, e.g. the main diagonal has zeros.

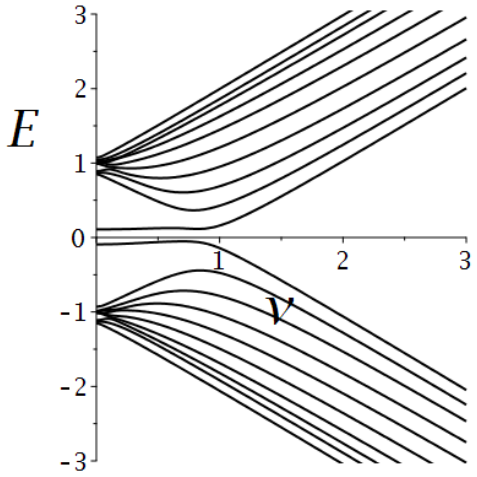

Figure 3 Plot of energies E as a function of intracell hopping v for fixed intercell hopping $w = 1$ for $N = 10$ unit cells. The system has random on-site energies chosen within the range -0.2 to $+0.2$. Only results for one realisation of disorder are shown.

Fig.3 shows the eigenenergies E as a function of intracell hopping v for fixed intercell hopping $w = 1$ for $N = 10$ unit cells. Now there are randomly chosen onsite energies which simulates the effect of disorder. As the disorder breaks chiral symmetry, it tends to lead to an energy gap between the states near $E = 0$ for $v < w$. What would happen if the hopping parameters v and w were disordered, rather than the onsite energies? When considering disorder, it's perhaps not appropriate to only consider one realisation of disorder (as in Fig.3), but to average properties over many different realisations of disorder (and, perhaps, to consider fluctuations, e.g. variance, etc). One often considers the disorder-averaged density of states (global and local).

Open-ended part

Please note:

1. **The aim is for your group to do its own, original calculations.** A literature review and, perhaps, reproduction of other people's results may be important steps along the way, but these are not the final aim.
2. This topic ran for the second time last year. It is a current hot topic of research, so finding something new to do in all the other activity could be difficult. The study of disorder and/or the effect of long-range hoppings (in certain models) may be novel. This is probably the topic with the most scope for some analytic (pen and paper) calculations, although numerics will still be very important.

Ideas include:

- What's the role of long-range hoppings and/or disorder in the SSH model? This has already been considered to some extent, see, e.g. [3,4].

- Ref [4] (among many others) considered solitons (topological domain walls) in the SSH model. An alternative, related model is the CDW model [5]. It might be interesting to compare the role of long-range hoppings in the two models.
- Two coupled SSH chains, e.g. [6]. What's the role of long-range hoppings and/or disorder in this system?
- Derive tight-binding models in wavevector space (often just a 2×2 matrix) and use them to determine the band structure and topological invariants (Berry curvature, Chern number). Use the tight-binding model in real space to consider the effect of disorder and its influence on edge states.
- Two-dimensional systems e.g. honeycomb lattice (graphene), Lieb lattice, Kagome lattice, square-octagon lattice, ruby lattice.
- The square lattice with staggered hoppings (i.e. generalisation of the SSH model) is unusual because the Berry curvature and Chern number are zero, but there are still topological invariants (Zak phase/polarisation) [7,8,9].
- Role of disorder and/or a domain wall in the square lattice with staggered hoppings.
- Quantum spin Hall effect in graphene, i.e. graphene with spin-orbit coupling, see Eq.6 and Fig.1 in [10].
- The Kitaev chain (model of topological superconductivity and Majorana fermions) [11,12].
- Non-Hermitian models, e.g. [13]. For a recent paper with a large bibliography, see [14].

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