Helical Ladder Model

Jack Crewse

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1 Introduction

The goal in this set of notes is to understand the simulation of a 'helical ladder' system - consisting of a two atom unit cell which features screw dislocations along an axis which extends to infinity (e.g. similar to the DNA double helix) - using the `kwant` quantum transport simulation package. This simulation is intended to be the starting point for understanding the simulation of general helical materials consisting of 'bulk' 2D materials stacked with a twist angle between layers.

2 Simple Ladder Model

To get started, we first simulate a simple ladder system (two atom units cell without the screw dislocation). This has a relatively simple Hamiltonian (in atomic units $\hbar = m = c = 1$) in the tight-binding approximation

$$H_{SL} = u \sum_{i,j} |i,j\rangle\langle i,j| \tag{1}$$

$$- t \sum_{i,j} \left[|i,j\rangle\langle i,j+1| + |i,j+1\rangle\langle i,j| \right] \tag{2}$$

$$- v \sum_{i,j} \left[|i,j\rangle\langle i+1,j| + |i+1,j\rangle\langle i,j| \right] \tag{3}$$

$$- w \sum_{i} \left[|i,0\rangle\langle i+1,1| + |i+1,1\rangle\langle i,0| + |i,0\rangle\langle i-1,1| + |i-1,1\rangle\langle i,0| \right]. \tag{4}$$

The first term (1) accounts for on-site energies u, the second term (2) accounts for hopping along the y-axis (within the layer) with hopping integral t, the third term (3) accounts for hopping along the x-axis (between layers) with hopping integral v, and the fourth term (4) accounts for 'cross' hopping (i.e. next-nearest neighbors) with hopping integral w. A schematic of this system is shown in Figure 1 (left) along with the system as output by `kwant` (right).

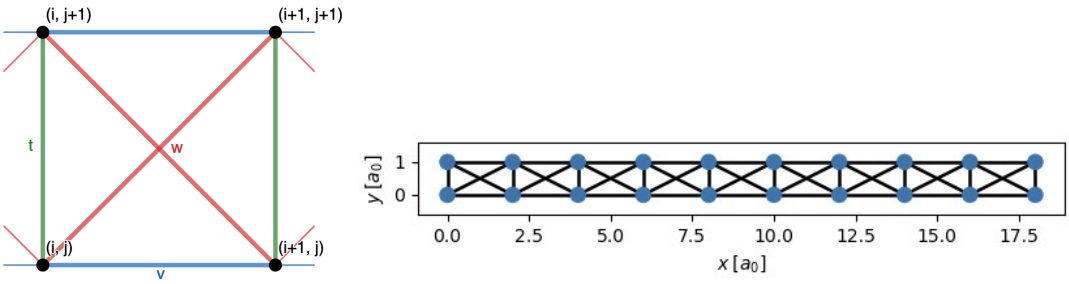

Figure 1: Left: A schematic of a few sites of the ladder system defining hopping and site-labeling conventions. Right: A finite length example of the simple ladder system as output from kwant. Lengths in units of the Bohr radius.

2.1 Spectrum and wavefunctions: Finite-system

First we consider the spectrum ϵ_n and wavefunctions $\Psi_n(x, y)$ of a few of the lowest states for the simplest case of a finite-length ladder model. Figure 2 shows the eigenvalue spectrum and wave functions of the lowest calculated eigenenergies. The lowest state is a nodeless state and the increase in energy corresponds to an increase in the number of nodes in the wavefunctions (or probability density $|\Psi|^2$).

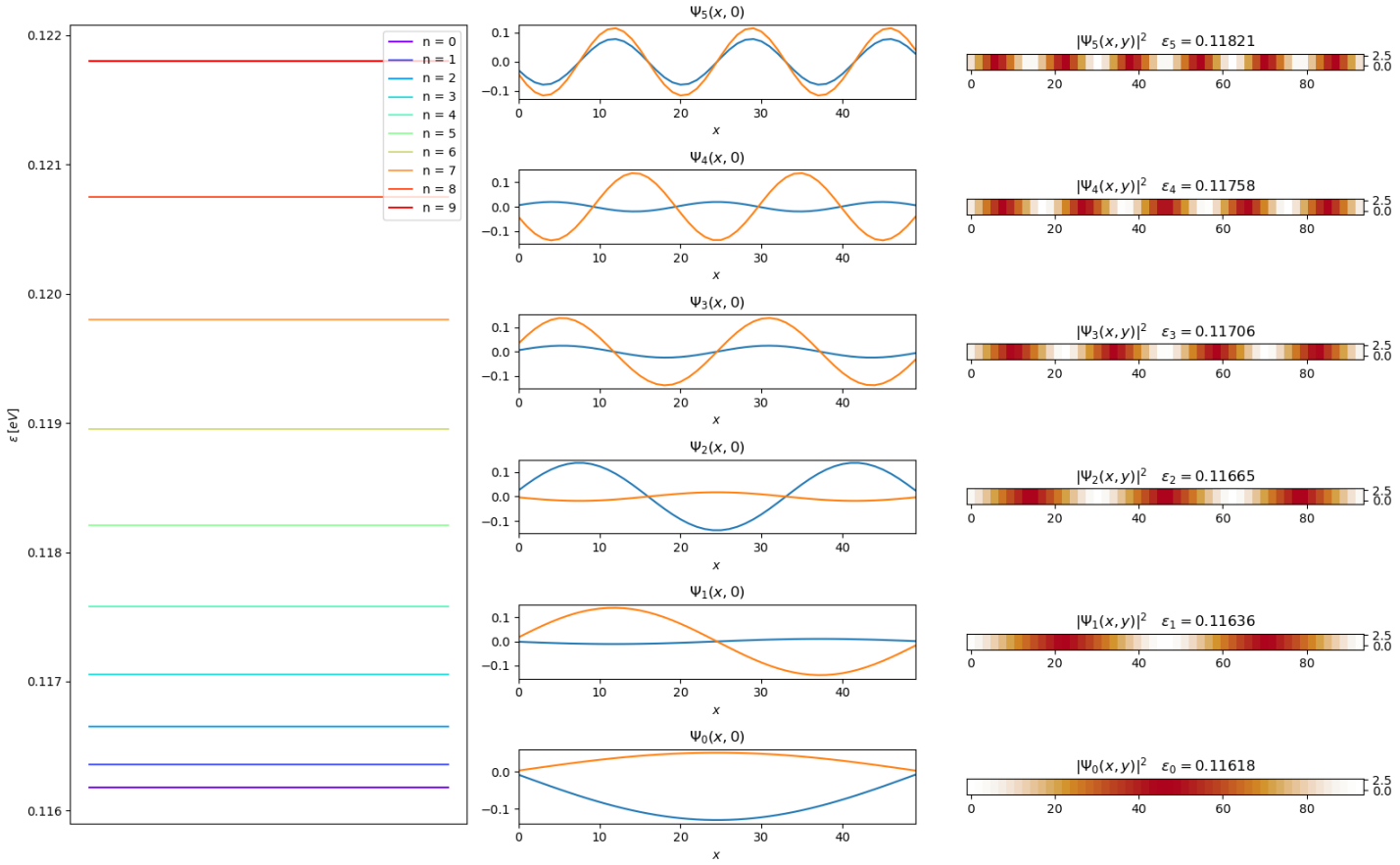

Figure 2: Left: Eigenvalue spectrum for the simple ladder model. Right: Probability density for the five lowest eigenenergies. Calculated from a system with lattice constants $a = b = 1$, on-site energy $u = 5$, and hoppings $t = v = w = 1$.

2.2 Band Structure

We first consider the most basic case of this simple ladder system. A system with equal lattice constants $a = b = a_0$ ($a_0 =$ the Bohr radius) and with no cross hoppings $w = 0$ (i.e. only nearest-neighbor hopping). The band structure for this case can be seen in figure 1 (left). As we increase the intralayer hopping parameter t, we see that the separation between the valence and conduction bands begins to widen because the energy difference between the

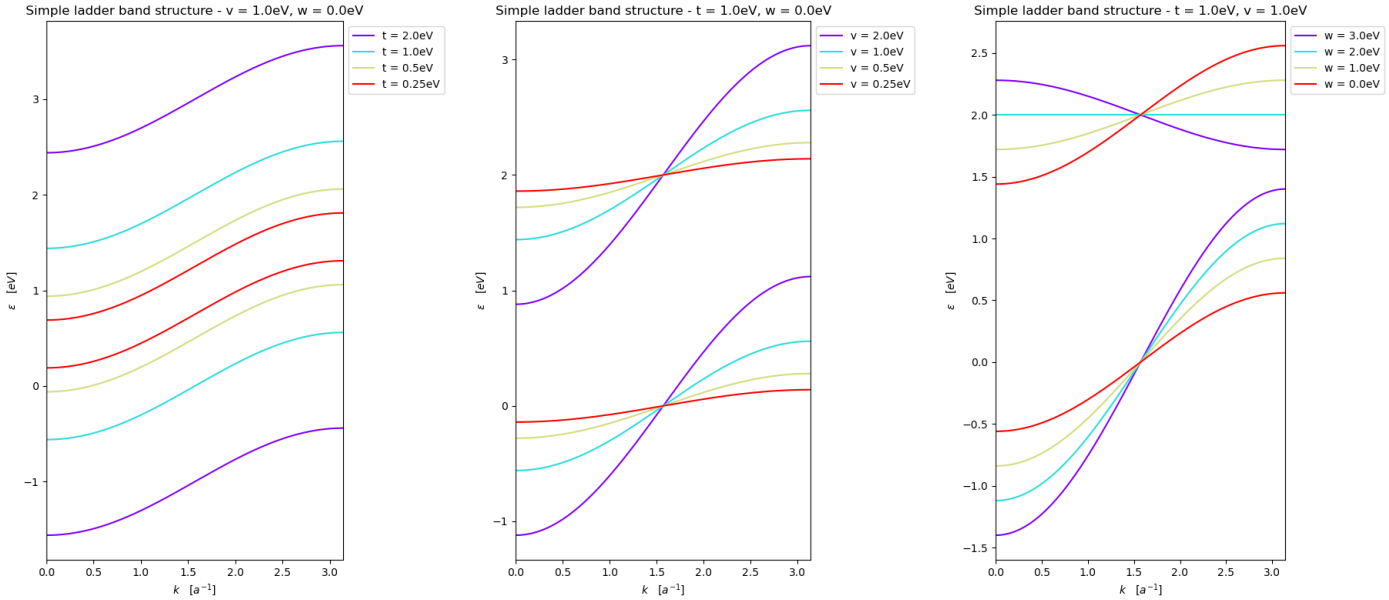

Figure 3: Band structure for the simple ladder model with a fixed interlayer hopping $v = 1$ and no cross hopping $w = 0$ is on the left. As the intralayer hopping parameter t is increased, the energies of both bands are increased the bandwidth and gap. The band structures for the same system but with a fixed intralayer hopping $t = 1$ and no cross hopping $w = 0$ is on the right. As the interlayer hopping parameter v is varied, you can see it evolve from a highly dispersed, high-bandwidth structure $v = 5.0$ to a nearly dispersion-less, two-level system $v = 0.25$ as the layers become effectively independent two atom systems.

3 Helical Ladder Model

Next, we want to introduce a twist angle ϕ into the simple ladder model along the x-axis. To implement this, instead of physically displacing the atomic locations (which is not straight-forward in `kwant`), as a first approximation we simply scale the tight-binding hopping parameters v and w (the in-plane hopping t is unaffected by the twist angle) according to the change in distance between the corresponding atoms that occurs in a rotation of ϕ. This approximation thus maps the hopping parameters as

$$v(\phi) \longrightarrow v/l_v(\phi) \tag{5}$$
$$w(\phi) \longrightarrow w/l_w(\phi) \tag{6}$$

where l_v and l_w represent the distances between atoms coupled via v and w, respectively. A simple vector analysis of helical ladder with twist angle ϕ shows

$$l_v(\phi) = \sqrt{\frac{a^2}{2}(1 - \cos\phi) + b^2} \tag{7}$$
$$l_w(\phi) = \sqrt{\frac{a^2}{2}(1 + \cos\phi) + b^2} \tag{8}$$

3.1 Spectrum and wavefunctions: Finite-system

Let's examine a finite helical ladder (i.e. with a twist angle) for a simple case of $\phi = \pi/2$. This creates a chain with each H_2 molecule being mutually perpendicular to the next in the chain. The results of this calculation are seen in Figure 4. Almost nothing changes about the states of the system other than seeing a slight increase in the eigenenergies. The wave functions and probability densities are almost identical. Why is this the case?

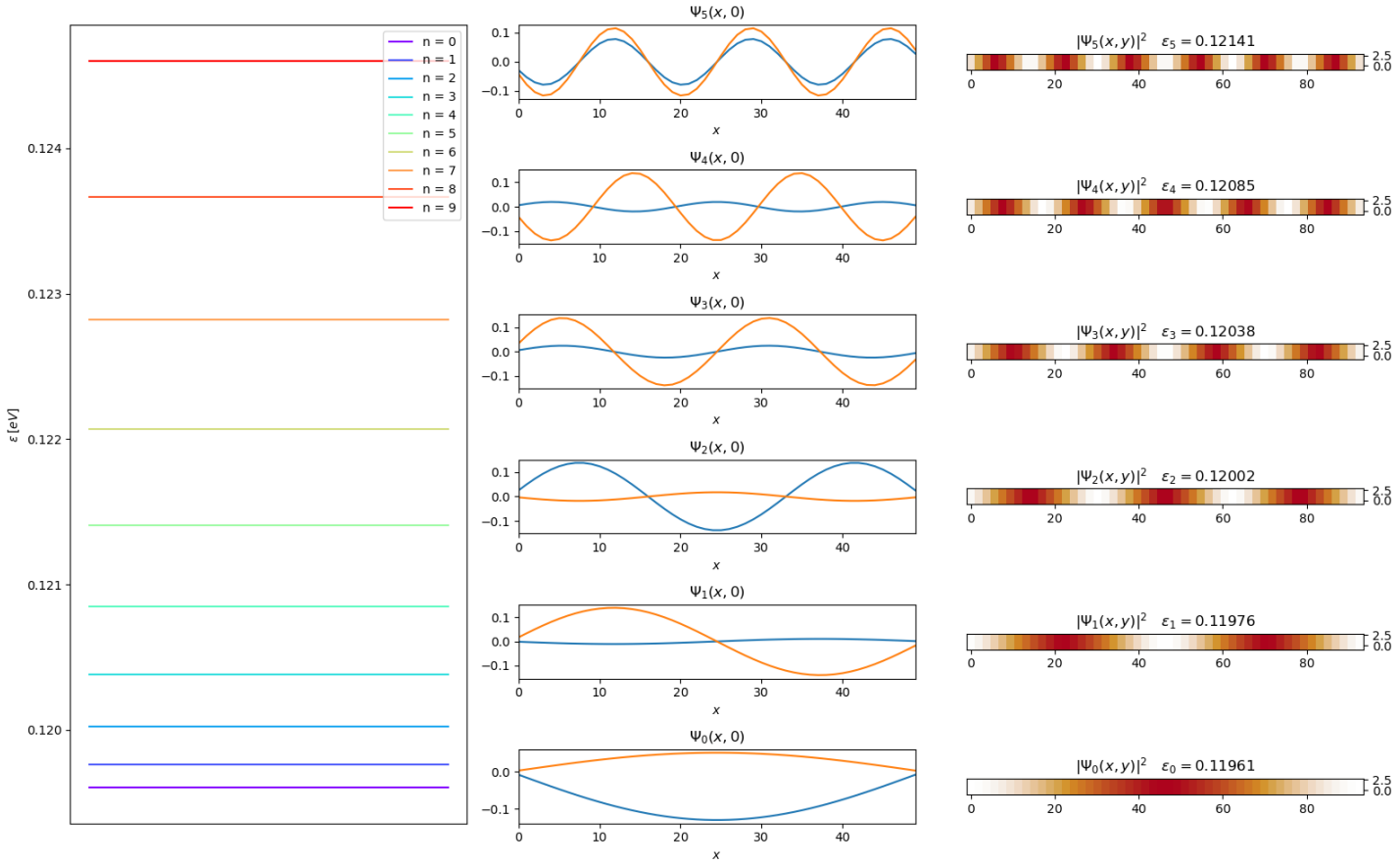

Figure 4: Helical ladder system with $\phi = \pi/2$

3.2 Band Structure

Now let's analyze the band structure of the helical ladder for a range of twist angles. Figure 5 shows the results. As we can see, the upper band is heavily affected by the twist angle. It begins to invert as we increase ϕ, becoming flat at $\phi = \pi/2, 3\pi/2$ (corresponding to a chain of mutually perpendicular H_2 molecules) and completely inverting at $\phi = \pi$ (corresponding to a chain of mutually parallel H_2 molecules. How is this different from the original system?)

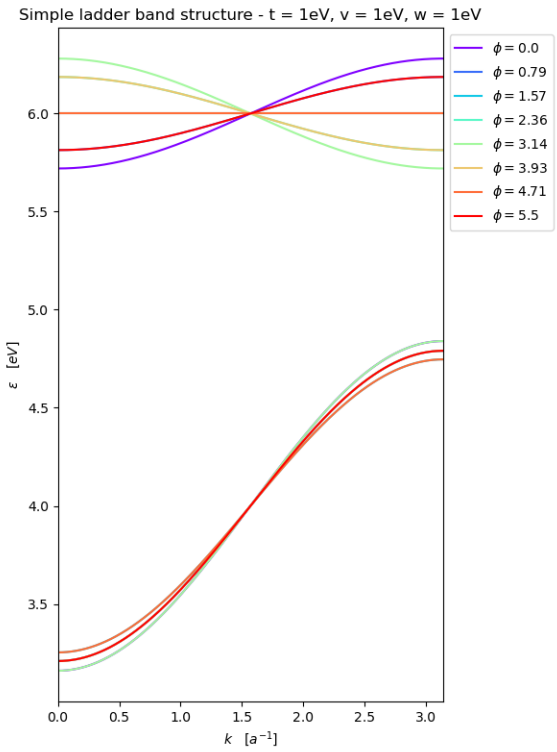

Figure 5: Band structure for a helical ladder for a range of twist angles.