Computational Tools for Quantum Many-Body Physics (WS 24/25)
Exercise Sheet 1

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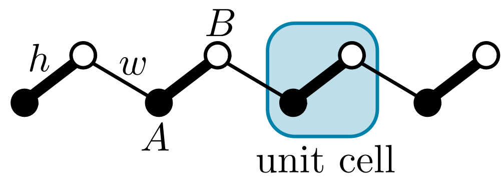
Online: Tue, 22 Oct 2024
Discussion: Tue, 05 Nov 2024

The goal of this exercise sheet is to gain experience in the modeling of non-interacting tight-binding Hamiltonians, and the calculation of some ground state as well as dynamical properties. As a paradigmatic example, we study the Su-Schrieffer-Heeger (SSH) Hamiltonian, that is a tight-binding model for spinless fermions hopping on a one-dimensional bipartite chain with staggered hopping amplitudes (see illustration below).



The Hamiltonian of the SSH model with L unit cells consisting of $n = 2$ orbitals A and B and open boundary conditions in second quantization reads as

$$H = h \sum_{j=1}^{L} \left(c_{j,A}^\dagger c_{j,B} + c_{j,B}^\dagger c_{j,A} \right) + w \sum_{j=1}^{L-1} \left(c_{j+1,A}^\dagger c_{j,B} + c_{j,B}^\dagger c_{j+1,A} \right) \tag{1}$$

where the fermionic operators $c_{j,A}^\dagger$, $c_{j,B}^\dagger$ create a fermion in the single-particle states $|j, A\rangle$, $|j, B\rangle$ localized in the j^{th} unit cell on A and B orbitals, respectively. Furthermore h is the hopping strength within a unit cell and w is the hopping strength between neighboring unit cells.

1. **Spectrum of the Hamiltonian**
   Fix $h = 1.0$. Calculate analytically and plot the single particle spectrum of the model (1) with periodic boundary conditions as a function of the lattice momentum k (i.e. the band structure), for the following values of w: $w = 0.5$, $w = 1.0$ and $w = 2.0$. What happens for $w = 1.0$?
   Compare the spectrum of (1) for the same values of w in the case of both periodic and open boundary conditions, now obtained numerically. What happens with open boundaries when $w = 2.0$ (in general $w > h$)?
   Plot the modulus squared of the two eigenstates close to 0 energy appearing with open boundaries at $w = 2.0$ (in general $w > h$).

   Hint: Looking at the limiting case $h = 0$, $w = 1.0$, the so-called *fully dimerized limit*, one can easily understand the presence of these eigenstates localized at the ends of the chain.

2. **Ground state correlation functions at half-filling**
   Consider now the half-filling situation for the model (1) with open boundaries, in which the number of fermions N_f in the bipartite chain is equal to half of the number of sites. The N_f-particle ground state of (1) is the Slater determinant $|\psi_0\rangle$. Calculate and plot

   $$G_{A,B}(j,\ell) = \langle \Psi_0 | c_{j,A}^\dagger c_{\ell,B} | \Psi_0 \rangle \tag{2}$$

   e.g. by fixing $j = L/4$ and sweeping ℓ from $L/4$ to $3L/4$, for h fixed to 1.0 and $w = 0.5$, $w = 1.0$, and $w = 2.0$. What changes in the behavior of $G_{A,B}(j,\ell)$ as w crosses the *phase transition* point $w = 1.0$?

   Hint: plot $|G_{A,B}(j,\ell)|$ in log-log scale. As seen in the first exercise, when $w = 1.0$ the energy gap between the two bands closes. At half-filling, this corresponds to a transition from an insulating to a metallic state, since as w becomes 1.0 the filled valence band touches the empty conduction band, and the excitation gap above $|\psi_0\rangle$ closes. Generally, the two-point function $G_{A,B}(j,\ell)$ for a metallic state has a *power-law* decay. Conversely when the system is insulating ($w \neq 1.0$ in the SSH model) the two-point functions exhibit an *exponential* decay.

This behavior is reflected in other correlation functions as well, as for instance the (connected part of the) density-density correlations:

$$C_{n,n}(j,\ell) = \langle \Psi_0 | n_j \, n_\ell | \Psi_0 \rangle - \langle \Psi_0 | n_j | \Psi_0 \rangle \langle \Psi_0 | n_\ell | \Psi_0 \rangle \tag{3}$$

where $n_j = n_{j,A} + n_{j,B} = c^\dagger_{j,A} c_{j,A} + c^\dagger_{j,B} c_{j,B}$. Calculate $C_{n,n}(j,\ell)$ using Wick's theorem and plot it in log-log scale for $w = 0.5$, $w = 1.0$ and $w = 2.0$ (again, one can fix $j = L/4$ and sweep ℓ from $L/4$ to $3L/4$).

One can extract a correlation length ξ from $C_{n,n}(j,\ell)$, by a fitting with a decay function

$$C_{n,n}(j,\ell) \propto \frac{e^{-\frac{|\ell - j|}{\xi}}}{|\ell - j|^\alpha} \ . \tag{4}$$

Plot the behavior of ξ as a function of w in the interval $w \in [0.5, 1.5]$. What happens at the transition point?

3. **Edge state population after a quench**
Consider the ground state $|\psi_0\rangle$ of (1) with open coundary conditions and L unit cells, and take the number of fermions in the system to be $L+1$, in the case $h = 1.0$, $w = 2.0$. Plot the density profile of $|\psi_0\rangle$ defined as

$$N(j) = \langle \Psi_0 | c^\dagger_{j,A} c_{j,A} + c^\dagger_{j,B} c_{j,B} | \Psi_0 \rangle \ . \tag{5}$$

Now suppose that at time $t = 0$ the system is in the state $|\psi_0\rangle$ and the value of w is suddently decreased to $w = 0.5$ (a *quench*). At times $t > 0$ the state $|\Psi_0\rangle$ will therefore evolve with an Hamiltonian $H_{[w=0.5]}$ of which $|\Psi_0\rangle$ is not a ground state anymore. Define the edge population n_{edge} to be

$$n_{\text{edge}} = c^\dagger_{1,A} c_{1,A} + c^\dagger_{1,B} c_{1,B} + c^\dagger_{2,A} c_{2,A} + c^\dagger_{2,B} c_{2,B} \tag{6}$$

and calculate its time evolution

$$N_{\text{edge}}(t) = \langle \Psi_0 | e^{iH_{[w=0.5]} t} \, n_{\text{edge}} \, e^{-iH_{[w=0.5]} t} | \Psi_0 \rangle \ . \tag{7}$$