Solutions to problem set 3 for "Topology in condensed matter"

Discussed in exercise class on December 5, 2023

1 SSH model

1. We will use Wolfram Mathematica for our numerical analysis. The plot of the eigenvalues can be produced using following code:

   ```
   SSHHamiltonian[t1_, t2_, L_] := (-1)*Table[
     If[Abs[i - j] == 1,
       If[Mod[(i + j - 1)/2, 2] == 1, t1, t2],
     0], {i, 1, L}, {j, 1, L}];
   Plot[Evaluate@Sort@Eigenvalues[SSHHamiltonian[t1, 1.0, 20]], {t1, 0, 2}]
   ```

   The result is shown on the Figure 1 (left).

2. In the lecture, it was shown that the localized zero energy state have amplitudes decaying as follows:

   $$a_n = \left(-\frac{t_1^*}{t_2}\right)^n a_0 \tag{1}$$

   with n being number of unit cell, which is related to the coordinate x as $n = x/2$. Thus:

   $$|\psi(x)| \propto e^{-x/\xi}, \quad \xi = \frac{2}{\ln(|t_2/t_1|)} \tag{2}$$

3. The overlap (and thus the energy splitting) between those localized states then can be estimated as

   $$\Delta E \sim \exp\left(-L/\xi\right) = \exp\left(-\frac{L}{2}\ln\left|\frac{t_2}{t_1}\right|\right) \tag{3}$$

   This scaling can be checked using following code:

   ```
   Gap[H_] := 2*Abs@First@Eigenvalues[H, -1,
     Method -> {"Arnoldi", "Criteria" -> "Magnitude", "Shift" -> 0}]
   Block[{L = 20, t2 = 1.0},
     Plot[{Log@Gap[SSHHamiltonian[t1, t2, L]], -L/2 Log[1/t1]}, {t1, 0, 1}]]
   ```

   The result is shown on the Figure 1 (right).

4. The generalization of the zero energy solution given in the lecture is straightforward:

   $$a_n = a_0 \prod_{k=1}^{n} \left(-\frac{t_1^{(k)*}}{t_2^{(k)}}\right) \Rightarrow \overline{\ln(|a_n|^2/|a_0|^2)} = -2n \times \overline{\ln|t_2/t_1|} \tag{4}$$

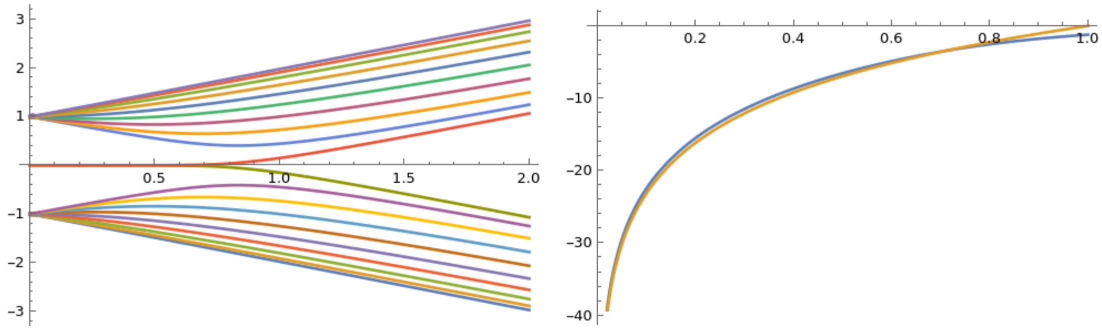

Figure 1: Numerical analysis of the SSH model with $L = 20$ sites at $t_2 = 1$. Left: all energy levels as a function of t_1. Right: logarithm of splitting between almost zero energy levels (blue) as a function of t_1 vs. predicted estimate.

2 Kitaev chain

1. Direct substitution of the inverse Fourier transform yields:

$$\hat{H} = \sum_p (-2t\cos p - \mu)\hat{c}_p^\dagger \hat{c}_p + \Delta \sum_p \left(\hat{c}_p \hat{c}_{-p} e^{-ip} + h.c.\right) \tag{5}$$

Let's "symmetrize" this as $\sum_p f(p) = \frac{1}{2}\sum_p (f(p) + f(-p))$, and then utilize the fermionic anti-commutation relations:

$$\begin{aligned}\hat{H} &= \frac{1}{2}\sum_p (-2t\cos p - \mu)\left(\hat{c}_p^\dagger \hat{c}_p + \hat{c}_{-p}^\dagger \hat{c}_{-p}\right) + \frac{\Delta}{2}\sum_p \left(\hat{c}_p \hat{c}_{-p} e^{-ip} + \hat{c}_{-p}\hat{c}_p e^{ip} + h.c.\right) \\ &= \frac{1}{2}\sum_p (-2t\cos p - \mu)\left(\hat{c}_p^\dagger \hat{c}_p + 1 - \hat{c}_{-p}\hat{c}_{-p}^\dagger\right) + \Delta \sum_p \left(\hat{c}_p \hat{c}_{-p}(-i\sin p) + h.c.\right) \\ &= \frac{1}{2}\sum_p (-2t\cos p - \mu) + \frac{1}{2}\sum_p \begin{pmatrix}\hat{c}_p^\dagger & \hat{c}_{-p}\end{pmatrix}\begin{pmatrix}-2t\cos p - \mu & 2i\Delta\sin p \\ -2i\Delta \sin p & 2t\cos p + \mu\end{pmatrix}\begin{pmatrix}\hat{c}_p \\ \hat{c}_{-p}^\dagger\end{pmatrix}\end{aligned} \tag{6}$$

which is precisely the required form with $h_0(p) = -2t\cos p - \mu$ and $\Delta(p) = 2i\Delta\sin p$. It is evident that:

$$\hat{H}_p^{(\mathrm{BdG})} = (-2t\cos p - \mu)\hat{\tau}_z - 2\Delta\sin p\,\hat{\tau}_y \Rightarrow \boldsymbol{d} = \begin{pmatrix}0 \\ -2\Delta\sin p \\ -2t\cos p - \mu\end{pmatrix} \tag{7}$$

2. Consider now Bogoliubov transformation:

$$\begin{cases}\hat{\psi}_p = u_p \hat{c}_p + v_p \hat{c}_{-p}^\dagger \\ \hat{\psi}_{-p}^\dagger = v_p' \hat{c}_p + u_p' \hat{c}_{-p}^\dagger\end{cases} \tag{8}$$

We have:

$$\{\hat{\psi}_p, \hat{\psi}_{-p}\} = \{u_p\hat{c}_p + v_p\hat{c}_{-p}^\dagger, v_p'^*\hat{c}_p^\dagger + u_p'^*\hat{c}_{-p}\} = u_p v_p'^* + v_p u_p'^* = 0 \tag{9}$$

$$\{\hat{\psi}_p, \hat{\psi}_p^\dagger\} = \{u_p\hat{c}_p + v_p\hat{c}_{-p}^\dagger, u_p^*\hat{c}_p + v_p^*\hat{c}_{-p}\} = |u_p|^2 + |v_p|^2 = 1 \tag{10}$$

and similarly

$$\{\hat{\psi}_p^\dagger, \hat{\psi}_{-p}^\dagger\} = u_p^* v_p' + v_p^* u_p' = 0 \tag{11}$$

$$\{\hat{\psi}_{-p}, \hat{\psi}_{-p}^\dagger] = |u_p'|^2 + |v_p'|^2 = 1 \tag{12}$$

These 4 conditions are indeed equivalent to the unitarity condition for $\hat{U}_p$:

$$\hat{U}_p\hat{U}_p^\dagger = \begin{pmatrix}|u_p|^2 + |v_p|^2 & u_p'^* v_p + v_p'^* u_p \\ u_p^* v_p' + v_p^* u_p' & |u_p'|^2 + |v_p'|^2\end{pmatrix} = \begin{pmatrix}1 & 0 \\ 0 & 1\end{pmatrix} \tag{13}$$

The eigenvalues of the Hamiltonian $\hat{H}_p^{(\mathrm{BdG})}$ are given by $\pm E_p$, with

$$E_p = |\boldsymbol{d}(\boldsymbol{p})| = \sqrt{h_0^2(p) + |\Delta(p)|^2} = \sqrt{(2t\cos p + \mu)^2 + \Delta^2 \sin^2 p} \tag{14}$$

The gap closes at $\Delta \sin p = 0$ and $2t\cos p + \mu = 0$, thus we have either:

$$\Delta = 0, \quad |\mu| < 2|t| \Rightarrow \cos p^* = -\frac{\mu}{2t} \tag{15}$$

$$p = 0, \quad \mu = -2t \tag{16}$$

$$p = \pi, \quad \mu = 2t \tag{17}$$

3. For $t = 1$, there are four topological phases:

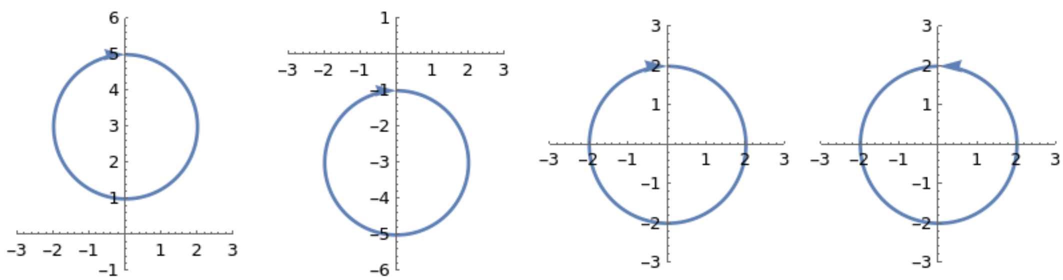

Figure 2: Winding number calculation for Kitaev chain for phases $(a) - (d)$. Plotted: trajectory of vector $(d_y(p), d_z(p))$ for $p \in [-\pi, \pi]$.

   (a) $\mu < -2$, $W = 0$.
   (b) $\mu > 2$, $W = 0$.
   (c) $\mu \in [-2, 2], \quad \Delta > 0$, $W = -1$.
   (d) $\mu \in [-2, 2], \quad \Delta < 0$, $W = +1$.

4. We have:

$$\hat{S}_n^+ \hat{S}_{n+1}^- = \hat{c}_n^\dagger \exp\left(-i\pi \sum_{k=0}^{n-1} \hat{c}_k^\dagger \hat{c}_k\right) \exp\left(i\pi \sum_{k=0}^{n} \hat{c}_k^\dagger \hat{c}_k\right) \hat{c}_{n+1} = \hat{c}_n^\dagger e^{i\pi \hat{c}_n^\dagger \hat{c}_n} \hat{c}_{n+1} \tag{18}$$

Since eigenvalues of $\hat{c}_n^\dagger \hat{c}_n = \{0, 1\}$, thus $\exp\left(i\pi \hat{c}_n^\dagger \hat{c}_n\right) \equiv 1 - 2\hat{c}_n^\dagger \hat{c}_n$:

$$\hat{S}_n^+ \hat{S}_{n+1}^- = \hat{c}_n^\dagger (1 - 2\hat{c}_n^\dagger \hat{c}_n) \hat{c}_{n+1} = \hat{c}_n^\dagger \hat{c}_{n+1} \tag{19}$$

Consider its hermitian conjuate: $\hat{S}_n^- \hat{S}_{n+1}^+ = \hat{c}_{n+1}^\dagger \hat{c}_n = -\hat{c}_n \hat{c}_{n+1}^\dagger$. Next we consider:

$$\hat{S}_n^- \hat{S}_{n+1}^- = \exp\left(i\pi \sum_{k=0}^{n-1} \hat{c}_k^\dagger \hat{c}_k\right) \hat{c}_n \exp\left(i\pi \sum_{k=0}^{n} \hat{c}_k^\dagger \hat{c}_k\right) \hat{c}_{n+1} = \hat{c}_n \exp\left(2\pi i \sum_{k=0}^{n-1} \hat{c}_k^\dagger \hat{c}_k\right) \exp\left(i\pi \hat{c}_n^\dagger \hat{c}_n\right) \hat{c}_{n+1} \tag{20}$$

Again, since eigenvalues of $\hat{c}_k^\dagger \hat{c}_k = \{0, 1\}$, thus $\exp(2\pi i \hat{c}_k^\dagger \hat{c}_k) \equiv 1$ and $\exp\left(i\pi \hat{c}_n^\dagger \hat{c}_n\right) = 2\hat{c}_n \hat{c}_n^\dagger - 1$, and we are left with:

$$\hat{S}_n^- \hat{S}_{n+1}^- = \hat{c}_n (2\hat{c}_n \hat{c}_n^\dagger - 1) \hat{c}_{n+1} = -\hat{c}_n \hat{c}_{n+1} \tag{21}$$

Finally, its hermitian conjugate completes the proof. This allows us to rewrite the Kitaev Hamiltonian as follows:

$$\hat{H} = -\sum_n \left[t(\hat{S}_n^+ \hat{S}_{n+1}^- + h.c.) + \mu\left(\hat{S}_n^z + \frac{1}{2}\right) + \Delta(\hat{S}_n^- \hat{S}_{n+1}^- + h.c.) \right]$$
$$= -\sum_n \left[2(t + \Delta)\hat{S}_n^x \hat{S}_{n+1}^x + 2(t - \Delta)\hat{S}_n^y \hat{S}_{n+1}^y + \mu\left(\hat{S}_n^z + \frac{1}{2}\right) \right] \tag{22}$$

3 AKLT model

1. First we note that:

$$\sum_M \hat{A}^{(M)} |M\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} -|0\rangle & \sqrt{2}\,|+1\rangle \\ -\sqrt{2}\,|-1\rangle & |0\rangle \end{pmatrix} \tag{23}$$

   and thus matrix multiplication proves the first statement. The total $\hat{S}^z$ for states (1,1) and (2,2) yields zero, thus one only needs to check that they are orthogonal to $|0\rangle$; the total $\hat{S}^z$ for state (1,2) is $+1$, thus we only need to check that it's orthogonal to $|1\rangle$; and finally the total $\hat{S}^z$ for state (2,1) is -1, thus we only need to check that it's orthogonal to $|-1\rangle$. These three checks are straightforward.

2. The transfer-matrix has four eigenvectors:

$$T_1 = +1 \Rightarrow |v_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad T_2 = -\frac{1}{3} \Rightarrow |v_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} \tag{24}$$

$$T_3 = -1/3 \Rightarrow |v_3\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad T_4 = -1/3 \Rightarrow |v_4\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \tag{25}$$

   and thus

$$\hat{T}^n = T_1^n |v_1\rangle \langle v_1| + T_2^n |v_2\rangle \langle v_2| + T_3^n |v_3\rangle \langle v_3| + T_4^n |v_4\rangle \langle v_4| = \begin{pmatrix} \frac{1}{2}(1+\lambda^n) & 0 & 0 & \frac{1}{2}(1-\lambda^n) \\ 0 & \lambda^n & 0 & 0 \\ 0 & 0 & \lambda^n & 0 \\ \frac{1}{2}(1-\lambda^n) & 0 & 0 & \frac{1}{2}(1+\lambda^n) \end{pmatrix} \tag{26}$$

   with $\lambda = -1/3$. which gives the desired result. For normalization we thus have:

$$\langle \text{AKLT}|\text{AKLT}\rangle = \text{Tr}\hat{T}^N = 1 + 3\lambda^N \to 1 \tag{27}$$

3. The direct calculation yields:

$$\left\langle \hat{S}_0^z \hat{S}_r^z \right\rangle \underset{N\to\infty}{=} \text{Tr}(\hat{Z}\hat{T}^{r-1}\hat{Z}\hat{T}^{N-r-1}) = \frac{4}{3} \cdot \left(\lambda^r + \lambda^{N-r}\right) \to \frac{4}{3}\lambda^r \tag{28}$$

   which is exponentially decaying.

4. Finally, the calculation for the string order parameter yields:

$$\left\langle \hat{S}_0^z \exp\left(i\pi \sum_{k=1}^{r-1} \hat{S}_k^z\right) \hat{S}_r^z \right\rangle = \text{Tr}(\hat{Z}\hat{T}_S^{r-1}\hat{Z}\hat{T}^{N-r-1}) = -\frac{4}{9} - 4\lambda^N \to -\frac{4}{9} \tag{29}$$