Diatomic tight binding chain

(a) The Heisenberg equation of motion is given by:

$$\frac{d}{d\tau}(c_i^\dagger c_{i+1}) = i[H, c_i^\dagger c_{i+1}],$$

where H is the Hamiltonian.

The Hamiltonian is:

$$H = -t\sum_{j=1}^{N}\left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j\right) + v_a\sum_{j=1}^{N/2} n_{2j-1} + v_b\sum_{j=1}^{N/2} n_{2j},$$

where $n_j = c_j^\dagger c_j$ is the number operator.

We want to compute the commutator $[H, c_i^\dagger c_{i+1}]$. We will consider the contributions from the hopping and on-site potential terms separately.

First,

$$\begin{aligned}
[c_j^\dagger c_{j+1}, c_i^\dagger c_{i+1}] &= [c_j^\dagger, c_i^\dagger c_{i+1}]c_{j+1} + c_j^\dagger[c_{j+1}, c_i^\dagger c_{i+1}] \\
&= c_i^\dagger[c_j^\dagger, c_{i+1}]c_{j+1} + [c_j^\dagger, c_i^\dagger]c_{i+1}c_{j+1} + c_j^\dagger c_i^\dagger[c_{j+1}, c_{i+1}] + c_j^\dagger[c_{j+1}, c_i^\dagger]c_{i+1} \\
&= c_i^\dagger(2c_j^\dagger c_{i+1} - \delta_{i+1,j})c_{j+1} - 2c_i^\dagger c_j^\dagger c_{i+1}c_{j+1} \\
&+ c_j^\dagger c_i^\dagger(-2c_{i+1}c_{j+1}) + c_j^\dagger(-2c_i^\dagger c_{j+1} + \delta_{i,j+1})c_{i+1} \\
&= -\delta_{i+1,j}c_i^\dagger c_{j+1} + \delta_{i,j+1}c_j^\dagger c_{i+1}.
\end{aligned} \tag{1}$$

Similarly,

$$[c_{j+1}^\dagger c_j, c_i^\dagger c_{i+1}] = \delta_{i,j}c_{j+1}^\dagger c_{i+1} - \delta_{i+1,j+1}c_i^\dagger c_j. \tag{2}$$

Now,

$$\begin{aligned}
[\sum_j c_j^\dagger c_{j+1}, c_i^\dagger c_{i+1}] &= -\sum_j \delta_{i+1,j}c_i^\dagger c_{j+1} + \sum_j \delta_{i,j+1}c_j^\dagger c_{i+1} \\
&= -c_i^\dagger c_{i+2} + c_{i-1}^\dagger c_{i+1}
\end{aligned} \tag{3}$$

and

$$\begin{aligned}
[\sum_j c_{j+1}^\dagger c_j, c_i^\dagger c_{i+1}] &= -\sum_j \delta_{i,j}c_{j+1}^\dagger c_{i+1} - \sum_j \delta_{i+1,j+1}c_i^\dagger c_j \\
&= -c_i^\dagger c_i + c_{i+1}^\dagger c_{i+1}.
\end{aligned} \tag{4}$$

Combining

$$[\sum_{j=1}^{N}\left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j\right), c_i^\dagger c_{i+1}] = -c_i^\dagger c_{i+2} + c_{i-1}^\dagger c_{i+1} - n_i + n_{i+1}. \tag{5}$$

On the other hand,

$$[c_j^\dagger c_j, c_i^\dagger c_{i+1}] = \delta_{i,j} c_j^\dagger c_{i+1} - \delta_{i+1,j} c_i^\dagger c_j. \tag{6}$$

and thus

$$\begin{aligned}
[\sum_j c_{2j-1}^\dagger c_{2j-1}, c_i^\dagger c_{i+1}] &= \sum_j \delta_{i,2j-1} c_{2j-1}^\dagger c_{i+1} - \sum_j \delta_{i+1,2j-1} c_i^\dagger c_{2j-1} \\
&= c_i^\dagger c_{i+1} - c_i^\dagger c_{i+1} = 0
\end{aligned} \tag{7}$$

and

$$[\sum_j c_{2j}^\dagger c_{2j}, c_i^\dagger c_{i+1}] = 0. \tag{8}$$

Therefore,

$$[H, c_i^\dagger c_{i+1}] = -t(-c_i^\dagger c_{i+2} + c_{i-1}^\dagger c_{i+1} - n_i + n_{i+1}). \tag{9}$$

Final Equation of Motion

Combining both contributions, the equation of motion for $c_i^\dagger c_{i+1}$ is:

$$\frac{d}{d\tau}(c_i^\dagger c_{i+1}) = it(c_i^\dagger c_{i+2} - c_{i-1}^\dagger c_{i+1} + n_i - n_{i+1}).$$

(b) **Band structure**

(i) Using the a and b operators we write

$$\begin{aligned}
H &= -t \sum_{j=1}^{N/2} \left(a_j^\dagger b_j + b_j^\dagger a_j + a_{j+1}^\dagger b_j + b_{j+1}^\dagger a_j \right) + v_a \sum_{j=1}^{N/2} a_j^\dagger a_j + v_b \sum_{j=1}^{N/2} b_j^\dagger b_j \\
&= -\frac{2t}{N} \sum_{\#k,k'} \sum_j \left[a_k^\dagger b_{k'} + b_k^\dagger a_{k'} + a_k^\dagger b_{k'} e^{-2ik} + b_k^\dagger a_{k'} e^{2ik'} \right] e^{-2i(k-k')j} \\
&\quad + v_a \sum_{\#k} a_k^\dagger a_k + v_b \sum_{\#k} b_k^\dagger b_k \\
&= -\frac{2t}{N} \sum_{k,k'} \frac{N}{2} \delta_{k,k'} \left[a_k^\dagger b_{k'} + b_k^\dagger a_{k'} + a_k^\dagger b_{k'} e^{-2ik} + b_k^\dagger a_{k'} e^{2ik'} \right] + v_a \sum_{\#k} a_k^\dagger a_k + v_b \sum_{\#k} b_k^\dagger b_k \\
&= -t \sum_{\#k} \left[(1 + e^{-2ik}) a_k^\dagger b_k + (1 + e^{+2ik}) b_k^\dagger a_k \right] + v_a \sum_{\#k} a_k^\dagger a_k + v_b \sum_{\#k} b_k^\dagger b_k \\
&= \sum_{\#k} \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} v_a & -t(1 + e^{-2ik}) \\ -t(1 + e^{+2ik}) & v_b \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}.
\end{aligned} \tag{10}$$

The fourth equality is the expression of the Hamiltonian in momentum space. One should be careful not to forget $a_{j+1}^\dagger b_j + b_{j+1}^\dagger a_j$ in the first line, otherwise half of the hopping terms in the Hamiltonian could be missed.

(ii) See the last line in (10).

(iii) $\mathcal{H}(k)$ can be written as

$$\mathcal{H}(k) = \frac{v_a + v_b}{2} \mathbf{I} - t \left[1 + \cos(2k) \right] \sigma^x - t \sin(2k) \sigma^y + \frac{v_a - v_b}{2} \sigma^z. \tag{11}$$

Therefore,

$$
\begin{aligned}
|h_k| &= \sqrt{t^2\left[1+\cos(2k)\right]^2 + t^2\sin(2k)^2 + \left(\frac{v_a - v_b}{2}\right)^2} \\
&= \sqrt{2t^2 + 2t^2\cos(2k) + \left(\frac{v_a - v_b}{2}\right)^2} \\
&= \sqrt{4t^2\cos(k)^2 + \left(\frac{v_a - v_b}{2}\right)^2}, \\
\theta_k &= \arccos\frac{v_a - v_b}{2|h_k|}, \\
\varphi_k &= \arctan\frac{\sin(2k)}{1+\cos(2k)},
\end{aligned} \tag{12}
$$

and the eigenvalues are $E_\pm(k) = \frac{v_a+v_b}{2} \pm |h_k|$, with the gap $\Delta = 2\min_k |h_k| = v_a - v_b$.

(c) $\{\beta_k, \beta^\dagger_{k'}\} = \{u^*_{11,k}a_k + u^*_{12,k}b_k, u_{11,k'}a^\dagger_{k'} + u_{12,k'}b^\dagger_{k'}\}$ where u_{ij} are the entry of the U matrix corresponding to i-th row and j-th column. Therefore,

$$
\{\beta_k, \beta^\dagger_{k'}\} = u^*_{11,k}u_{11,k'}\{a_k, a'^\dagger_k\} + u^*_{12,k}u_{12,k'}\{b_k, b'^\dagger_k\} = u^*_{11,k}u_{11,k'}\delta_{k,k'} + u^*_{12,k}u_{12,k'}\delta_{k,k'}. \tag{13}
$$

Therefore, $\{\beta_k, \beta^\dagger_{k'}\} = 0$ when $k \neq k'$. When $k = k'$, $\{\beta_k, \beta^\dagger_k\} = |u_{11,k}|^2 + |u_{12,k}|^2 = \sin^2\theta_k + \cos^2\theta_k = 1$. Thus, $\{\beta_k, \beta^\dagger_{k'}\} = \delta_{k,k'}$. Similarly, one can also find, $\{\alpha_k, \alpha^\dagger_{k'}\} = \delta_{k,k'}$.

(d) The lower band $E_-(k)$ has a minima at $k = 0$. By expanding $E_-(k)$ near $k = 0$, one finds

$$
E_-(k) = \frac{v_a + v_b}{2} - \sqrt{4t^2 + V} + \frac{2t^2}{\sqrt{4t^2+V}}k^2, \tag{14}
$$

where $V = \frac{v_a - v_b}{2}$ The free electron dispersion is given by $E_k = \hbar k^2/2m$. By comparing the two expressions one finds that the effective mass of electrons near the band minimum is

$$
m^* = \frac{\hbar\sqrt{4t^2+V}}{4t^2}.
$$

(e) By doing a similar calculation as above, one finds that

$$
E_-(k) = \frac{v_a + v_b}{2} - \sqrt{V} - \frac{2k^2t^2}{\sqrt{V}}. \tag{15}
$$

Thus, the effective mass for the lower band at $k = \pi/2$ is

$$
m^* = -\frac{\hbar\sqrt{V}}{4t^2}.
$$

Since an electron carries negative charge, the absence of an electron (a hole) behaves as if it has positive charge. When an electron has negative effective mass near the top of the lower band, the hole, which is essentially the absence of that electron, is assigned a positive effective mass. This is because the motion of the hole (as a vacancy) mirrors that of the electron.

(f) **Band structure**

(i) At $k = \pi/2$, $\theta_{k=\pi/2} = \arccos -1 = \pi$, hence

$$\begin{pmatrix} \beta_k \\ \alpha_k \end{pmatrix} = U^\dagger \begin{pmatrix} a_k \\ b_k \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} a_k \\ b_k \end{pmatrix} = \begin{pmatrix} b_k \\ a_k \end{pmatrix}. \tag{16}$$

The interaction between the electrons and holes most probably happens near the 'Fermi surface', which, in our case, is the point $k = \pi/2$, therefore, we would like to focus on this region.

(ii) We write

$$\begin{aligned}
\hat{U} &= u \sum_{j=1}^{N/2} (n_{2j} n_{2j+1} + n_{2j-1} n_{2j}) = u \sum_{j=1}^{N/2} n_{2j}(n_{2j+1} + n_{2j-1}) \\
&= u \sum_{j=1}^{N/2} b_j^\dagger b_j \left(a_j^\dagger a_j + a_{j+1}^\dagger a_{j+1} \right) \\
&= \frac{4u}{N^2} \sum_{j=1}^{N/2} \sum_{\#k,q,k',q'} e^{-i(k-q)2j} b_k^\dagger b_q (e^{-2i(k'-q')j} + e^{-2i(k'-q')(j+1)}) a_{k'}^\dagger a_{q'} \\
&= \frac{4u}{N^2} \sum_{\#k,q,k',q'} [\sum_{j=1}^{N/2} e^{-i(k+k'-q-q')2j}](1 + e^{2i(k'-q')}) b_k^\dagger b_q a_{k'}^\dagger a_{q'} \\
&= \frac{2u}{N} \sum_{\#k,q,k',q'} \delta_{k+k'-q-q',0} \left[1 + \cos(2k' - 2q') - i \sin(2k' - 2q')\right] b_k^\dagger b_q a_{k'}^\dagger a_{q'} \\
&\approx \frac{2u}{N} \sum_{\#k,q,k',q'} \delta_{k+k'-q-q',0} \left[1 + \cos(2k' - 2q') - i \sin(2k' - 2q')\right] \beta_k^\dagger \beta_q \alpha_{k'}^\dagger \alpha_{q'}.
\end{aligned} \tag{17}$$

Notice that $\sin(2k' - 2q')$ is odd w.r.t. $k' - q'$, or we simply write $U = (U + U^\dagger)/2$ since U is hermitian, we then can drop the sin terms. By using the trigonometry formula $\cos(2A) = 2\cos^2(A) - 1$, we reach the expression

$$\begin{aligned}
\hat{U} &= \frac{4u}{N} \sum_{\#k,q,k',q'} \delta_{k+k'-q-q',0} \cos^2(k' - q') \beta_k^\dagger \beta_q \alpha_{k'}^\dagger \alpha_{q'} \\
&\overset{k' \to q, \text{then } q \to k'+q}{=} \frac{4u}{N} \sum_{\#k,q,k'} \cos^2(k - k') \beta_k^\dagger \beta_{k'} \alpha_{k'+q}^\dagger \alpha_{k+q} \\
&= -\frac{4u}{N} \sum_{\#k,k',q} \cos^2(k - k') \alpha_{q+k} \beta_k^\dagger \beta_{k'} \alpha_{k'+q}^\dagger.
\end{aligned} \tag{18}$$

where in the last line anticommutation relation for fermions has been used:

$$\beta_k^\dagger \beta_q \alpha_{k'}^\dagger \alpha_{q'} = \beta_k^\dagger \beta_q (\delta_{q',k'} - \alpha_{q'} \alpha_{k'}^\dagger) = -\alpha_{q'} \beta_k^\dagger \beta_q \alpha_{k'}^\dagger + \underbrace{\delta_{q',k'} \beta_k^\dagger \beta_q}_{\text{neglected}}.$$

(iii) $E_{\text{shift}} = \frac{v_a + v_b}{2}$. After the energy shift, we can write

$$H = \sum_{\#k} \left(-E_k \alpha_k^\dagger \alpha_k + E_k \beta_k^\dagger \beta_k \right)$$

where $E_k = |h_k|$.

Then we need to deal with $(H + U) |\Psi_q\rangle = [\sum_{\#k} (-E_k \alpha_k^\dagger \alpha_k + E_k \beta_k^\dagger \beta_k) + U] |\Psi_q\rangle = (E_\Omega + \omega_q) |\Psi_q\rangle$. Let's divide the expression into three parts, and use the fact that $\alpha_k^\dagger |\Omega\rangle = 0$ and $\beta_k |\Omega\rangle = 0$ for any valid k:

- $$\begin{aligned}
&(\sum_{\#k} -E_k\alpha_k^\dagger\alpha_k)(\sum_{\#k} A_k^q\,\alpha_{q+k}\beta_k^\dagger\,|\Omega\rangle) = -\sum_{\#k,k'} E_kA_{k'}^q\alpha_k^\dagger\alpha_k\alpha_{q+k'}\beta_{k'}^\dagger\,|\Omega\rangle \\
&= \sum_{\#k,k'} E_kA_{k'}^q(-\alpha_{q+k'}\alpha_k^\dagger + \delta_{k,k'+q})\alpha_k\beta_{k'}^\dagger\,|\Omega\rangle \\
&= \sum_{\#k'} A_{k'}^q\alpha_{q+k'}\beta_{k'}^\dagger(-\sum_{\#k} E_k\alpha_k^\dagger\alpha_k\,|\Omega\rangle) + \sum_{\#k'} E_{k'+q}A_{k'}^q\alpha_{k'+q}\beta_{k'}^\dagger\,|\Omega\rangle \\
&= E_\Omega\,|\Psi_q\rangle + \sum_{\#k} E_{k+q}A_k^q\alpha_{k+q}\beta_k^\dagger\,|\Omega\rangle
\end{aligned} \tag{19}$$

- $$\begin{aligned}
&(\sum_{\#k} E_k\beta_k^\dagger\beta_k)(\sum_{\#k} A_k^q\,\alpha_{q+k}\beta_k^\dagger\,|\Omega\rangle) = \sum_{\#k,k'} E_kA_{k'}^q\beta_k^\dagger\beta_k\alpha_{q+k'}\beta_{k'}^\dagger\,|\Omega\rangle \\
&= \sum_{\#k,k'} E_kA_{k'}^q\beta_k^\dagger(\beta_{k'}^\dagger\beta_k - \delta_{k,k'})\alpha_{k'+q}\,|\Omega\rangle \\
&= 0 - \sum_{\#k} E_kA_k^q\beta_k^\dagger\alpha_{k+q}\,|\Omega\rangle \\
&= \sum_{\#k} E_kA_k^q\alpha_{k+q}\beta_k^\dagger\,|\Omega\rangle
\end{aligned} \tag{20}$$

- $$\begin{aligned}
U\,|\Psi_q\rangle &= -\frac{u}{4N}\sum_{\#k,k',q'} \cos^2(k-k')\alpha_{k+q'}\beta_k^\dagger\beta_{k'}\alpha_{k'+q'}^\dagger\sum_{\#p} A_p^q\alpha_{p+q}\beta_p^\dagger\,|\Omega\rangle \\
&= -\frac{u}{4N}\sum_{\#k,k',q',p} A_p^q\cos^2(k-k')\alpha_{k+q'}\beta_k^\dagger\beta_{k'}\alpha_{k'+q'}^\dagger\alpha_{p+q}\beta_p^\dagger\,|\Omega\rangle \\
&= -\frac{u}{4N}\sum_{\#k,k',q',p} A_p^q\cos^2(k-k')\alpha_{k+q'}\beta_k^\dagger\beta_{k'}\beta_p^\dagger(\delta_{k'+q',p+q} - \underbrace{\alpha_{p+q}\alpha_{k'+q'}^\dagger}_{\text{gives } 0})\,|\Omega\rangle \\
&= -\frac{u}{4N}\sum_{\#k,k',p} A_p^q\cos^2(k-k')\alpha_{k-k'+p+q}\beta_k^\dagger\beta_{k'}\beta_p^\dagger\,|\Omega\rangle \\
&= -\frac{u}{4N}\sum_{\#k,k',p} A_p^q\cos^2(k-k')\alpha_{k-k'+p+q}\beta_k^\dagger(\delta_{k',p} - \underbrace{\beta_p^\dagger\beta_{k'}}_{0})\,|\Omega\rangle \\
&= -\frac{u}{4N}\sum_{\#k,k'} A_{k'}^q\cos^2(k-k')\alpha_{k+q}\beta_k^\dagger\,|\Omega\rangle
\end{aligned} \tag{21}$$

Group the equations (19), (20) and (21) together and we will get

$$\begin{gathered}
E_\Omega\,|\Psi_q\rangle + \sum_{\#k}(E_{k+q}+E_k)A_k^q\alpha_{k+q}\beta_k^\dagger\,|\Omega\rangle - \frac{u}{4N}\sum_{\#k,k'} A_{k'}^q\cos^2(k-k')\alpha_{k+q}\beta_k^\dagger\,|\Omega\rangle = (E_\Omega+\omega_q)\,|\Psi_q\rangle \\
\sum_{\#k}\underbrace{\left[(E_{k+q}+E_k-\omega_q)A_k^q - \frac{u}{4N}\sum_{\#k'} A_{k'}^q\cos^2(k-k')\right]}_{=0}\alpha_{k+q}\beta_k^\dagger\,|\Omega\rangle = 0
\end{gathered} \tag{22}$$

From (22) we find our final results.

(iv) Given $\cos(k - k') \approx 1$, we write

$$\begin{aligned} (E_k + E_{k+q} - \omega_q)\, A_k^q &= \frac{4u}{N} \sum_{\#k'} A_{k'}^q \\ \frac{1}{4u} A_k^q &= \frac{1}{N} \frac{1}{E_k + E_{k+q} - \omega_q} \sum_{\#k'} A_{k'}^q \end{aligned} \tag{23}$$

Since (23) holds for all k, we can sum the equation over k on both sides, and get

$$\frac{1}{4u} \times \cancel{\textstyle\sum_{\#k} A_k^q} = \frac{1}{N} \sum_{\#k} \frac{1}{E_k + E_{k+q} - \omega_q} \times \cancel{\textstyle\sum_{\#k'} A_{k'}^q} \tag{24}$$

and we reach

$$\frac{1}{4u} = \frac{1}{N} \sum_{\#k} \frac{1}{E_k + E_{k+q} - \omega_q}\ . \tag{25}$$

(v) **(Optional)** Check the *Mathematica* notebook.