Problem 5.1 One-Dimensional Model of a Semiconductor

The Hamilton operator is $H_1 = H_0 + V$ where

$$H_0 = -\mathrm{t}\sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right), \tag{1}$$

$$V = v\sum_i (-1)^i\, c_i^\dagger c_i. \tag{2}$$

(a) Let us consider the case $v = 0$. We write

$$c_j^\dagger = \frac{1}{\sqrt{N}}\sum_k e^{ikj} c_k^\dagger, \qquad\qquad c_j = \frac{1}{\sqrt{N}}\sum_k e^{-ikj} c_k, \tag{3}$$

where $k \in [-\pi, \pi)$ and $kN = 2\pi n$, $n \in \mathbb{Z}$, and $\mathrm{a} = 1$. The above expression is plugged into Eq. (1) and we obtain

$$H_0 = -\frac{\mathrm{t}}{N}\sum_{k,k',j}\left(e^{i[kj-k'(j+1)]} + e^{i[k(j+1)-ik'j]}\right) c_k^\dagger c_{k'} \tag{4}$$

$$= -\mathrm{t}\sum_{k,k'} c_k^\dagger c_{k'}\left(e^{-ik'} + e^{ik}\right)\underbrace{\frac{1}{N}\sum_j e^{i(k-k')j}}_{\delta_{k,k'}} = \sum_k \underbrace{(-2\mathrm{t}\cos k)}_{\epsilon_k}\, c_k^\dagger c_k\ , \tag{5}$$

where we have made use of the Bravais sum.[1]

Let us define the following one-particle state: $|\phi_k\rangle = c_k^\dagger|0\rangle$ where $|0\rangle$ is the vacuum. It fulfills

$$c_k^\dagger c_k|\phi_k\rangle = c_k^\dagger c_k c_k^\dagger|0\rangle = c_k^\dagger(1 - c_k^\dagger c_k)|0\rangle = c_k^\dagger|0\rangle = |\phi_k\rangle, \tag{6}$$

and consequently

$$H_0|\phi_k\rangle = \epsilon_k|\phi_k\rangle. \tag{7}$$

Therefore, $|\phi_k\rangle$ is an eigenstate of the Hamilton operator. A similar procedure may be performed also with many-particle states $c_{k_1}^\dagger c_{k_2}^\dagger \ldots c_{k_n}^\dagger|0\rangle$.

(b) Let's consider now the case $v \neq 0$. Again, the expression (3) is plugged into V:

$$V = v\sum_{k,k'}\underbrace{\left[\frac{1}{N}\sum_j e^{i\pi j}\, e^{i(k-k')j}\right]}_{\delta_{k,k'+\pi}} c_k^\dagger c_{k'}\ , \tag{8}$$

where we have used the identity $(-1)^j \equiv e^{i\pi j}$ (for integer j). It follows that

$$H_1 = \sum_{k\in[-\pi/2,\pi/2]}{}' \left(\epsilon_k\, c_k^\dagger c_k + \epsilon_{k+\pi}\, c_{k+\pi}^\dagger c_{k+\pi} + v\, c_k^\dagger c_{k+\pi} + v\, c_{k+\pi}^\dagger c_k\right)\ . \tag{9}$$

[1]A more precise form of the Bravais sum is $\sum_j e^{i(k-k')j} = N\delta_{k,k'+G}$, where G may be an arbitrary reciprocal lattice vector (in our case $G = 2n\pi$). Thus, by restricting ourselves to the first Brillouin zone we obtain the result quoted in the main text.

From now on we will work only in the reduced Brillouin zone ($k \in [-\pi/2, \pi/2]$), for which the notation $\sum'$ stands. Note that

$$\epsilon_{k+\pi} = -2\mathrm{t}\cos(k+\pi) = 2\mathrm{t}\cos k = -\epsilon_k. \tag{10}$$

Introducing

$$\bar{c}_k = \begin{pmatrix} c_k \\ c_{k+\pi} \end{pmatrix} \tag{11}$$

the Hamilton operator is written in matrix form

$$H_1 = \sum_k{}' \bar{c}_k^\dagger \hat{H}_1 \bar{c}_k, \tag{12}$$

where

$$\hat{H}_1 = \begin{pmatrix} \epsilon_k & v \\ v & -\epsilon_k \end{pmatrix}. \tag{13}$$

We define new operators a_k and b_k according to

$$\bar{c}_k = \begin{pmatrix} c_k \\ c_{k+\pi} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ v_k & -u_k \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} = U\bar{\alpha}_k, \tag{14}$$

$$H_1 = \sum_k{}' \bar{\alpha}_k^\dagger U^\dagger \hat{H}_1 U \bar{\alpha}_k. \tag{15}$$

We can choose U such that $U^\dagger \hat{H}_1 U$ is diagonal. The energies are obtained from the secular equation

$$\det \begin{pmatrix} \epsilon_k - \lambda & v \\ v & -\epsilon_k - \lambda \end{pmatrix} = \lambda^2 - \epsilon_k^2 - v^2 = 0 \tag{16}$$

which has the solutions

$$\lambda = \pm\sqrt{\epsilon_k^2 + v^2} = \pm E_k. \tag{17}$$

Furthermore, one finds

$$u_k = \frac{v}{\sqrt{2E_k(E_k + \epsilon_k)}}, \qquad v_k = -\sqrt{\frac{E_k + \epsilon_k}{2E_k}}. \tag{18}$$

Finally, the Hamilton operator is written in the eigenbasis

$$H_1 = \sum_k{}' \left(-E_k\, a_k^\dagger a_k + E_k\, b_k^\dagger b_k\right). \tag{19}$$

(c) The band structure of the alternating chain is shown in Fig. 1. The gap between valence and conduction band is $\Delta = 2E_{\pm\pi/2} = 2v$. The ground state for $N/2$ electrons on the chain is given by

$$|\Omega\rangle = \prod_{k=-\pi/2}^{\pi/2} a_k^\dagger |0\rangle. \tag{20}$$

Compared to a) where we had a half filled band, we now have one fully filled band (due to the Brillouin zone reduction) with a finite gap for all kinds of excitations.

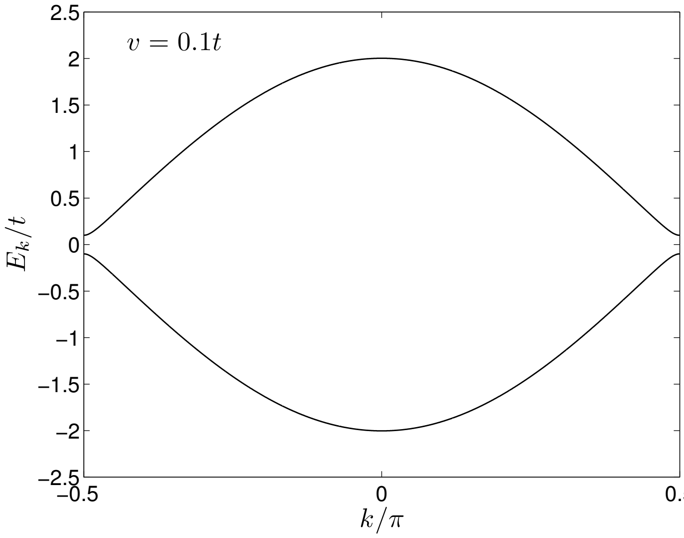

Figure 1: The two bands of the alternating chain.