Solid State Theory
Exercise 5

Problem 5.1 One-Dimensional Model of a Semiconductor

Let us consider electrons moving on a one-dimensional chain. We use the so-called tight-binding approximation. Thus, we assume that each atom has a localized electron state and that the electrons are able to hop between neighboring atoms. This hopping process describes the kinetic energy term.
It is most convenient to use a second-quantized language. For simplicity, we assume the electrons to be spinless fermions. Let c_i and $c_i^\dagger$ be the creation and annihilation operators for an electron at site i, respectively. The overlap integral between neighboring electron states is denoted by t. Then, the kinetic energy operator is written as

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

We assume that the chain contains N atoms and in the following we set the lattice constant $a = 1$. As a second step, we consider an alternating bipartite lattice which we model by a potential of the form

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

(a) Consider first the case $v = 0$. Show that the states created by

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

are eigenstates of H_0 with energy $\epsilon_k = -2\mathrm{t} \cos k$. Here, k belongs to the first Brillouin zone $[-\pi, \pi)$.

(b) For $v \neq 0$ the creation operators for the new eigenstates can be obtained by means of a so-called *Bogoliubov transformation* which we write as

$$a_k^\dagger = u_k c_k^\dagger + v_k c_{k+\pi}^\dagger, \qquad b_k^\dagger = v_k c_k^\dagger - u_k c_{k+\pi}^\dagger \tag{4}$$

where $u_k^2 + v_k^2 = 1$ (both u_k and v_k may be assumed to be real) for all k in the reduced Brillouin zone $[-\pi/2, \pi/2)$. Diagonalize the Hamiltonian and show that it can be written in the form

$$H_0 + V = \sum_{k \in [-\frac{\pi}{2}, \frac{\pi}{2})} \left(-E_k a_k^\dagger a_k + E_k b_k^\dagger b_k \right), \qquad E_k = \sqrt{\epsilon_k^2 + v^2}. \tag{5}$$

(c) Consider now the ground state of the half-filled chain ($N/2$ electrons). What is the difference between the cases (a) and (b)?