3. Consider a 1d chain, with a single tight-binding orbital on each site \( r = na \), where \( a \) is the lattice spacing and \( n \) is an integer. Ignoring spin, the quantum state corresponding to the tight-binding orbital at site \( r \) is denoted \( |r⟩ \). Suppose that, as shown in Fig. 3, the hopping matrix element on every “even” bond is \( t \), while on every “odd” bond it is \( t' \). Suppose the chain has a total of \( N \) sites, where \( N \) is even, and has periodic boundary conditions.

(a) Write down the tight-binding Hamiltonian in terms of \( |r⟩, t \) and \( t' \).

(b) Suppose we add electrons to the system until the number of electrons is the same as the number of lattice sites. (Do not forget about spin!) This situation is called half-filling, since we have half the maximum possible number of electrons.

Solve for the tight-binding band structure in the case \( t = t' \). Plot \( \epsilon_n(k) \) as a function of \( k \) in the Brillouin zone, and indicate which states are filled with electrons.

(c) Now consider \( t \neq t' \). Solve for the band structure and plot it. Again, indicate which states are filled by electrons (assuming half-filling, as before). \*Hint: You may find it helpful to think about how we solved a similar problem for 1d lattice vibrations. We considered a 1d harmonic chain with two atoms in each crystalline unit cell, where there were two different spring constants, and found both acoustic and optical vibration modes.

(d) What is the physical distinction between the ground states found above when (1) \( t = t' \) and (2) \( t \neq t' \)?

4. **Tight-binding band structure of graphene.**

Graphene can be modeled by a single tight-binding orbital on each site of the honeycomb lattice (Fig. 4a). If we call the honeycomb sites \( r \), and the corresponding orbital \( |r⟩ \), the tight-binding Hamiltonian is

\[
H_{TB} = -t \sum_{(rr')} \left[ |r⟩⟨r'| + |r'|⟨r⟩ \right],
\]

where the sum is over nearest-neighbor bonds of the honeycomb lattice.

As illustrated in Fig. 4a, the honeycomb lattice is a lattice with 2-site basis. The Bravais lattice vectors are \( R = n_1a_1 + n_2a_2 \), where \( a_1 = ax \) and \( a_2 = a[(1/2)x + (√3/2)y] \). Lattice sites can be labeled by the pair \( (R, i) \), where \( i = 1, 2 \) labels the two sites in the basis. So this means that the site \( r \) can be represented by a pair \( (R, i) \), and we can also write \( |r⟩ = |R, i⟩ \). This labeling will be helpful in solving this problem.

(a) Write down the primitive vectors of the reciprocal lattice, and draw the corresponding Brillouin zone.

(b) Express the tight-binding Hamiltonian in terms of the states \( |R, i⟩ \). Instead of a sum over bonds as above, you should express the Hamiltonian using a single sum over Bravais lattice vectors \( R \).

(c) Solve for the tight-binding band structure. You should find two bands. Plot the band structure along the line \( k_y = 0 \).

(d) Suppose, as in graphene, that we are at half-filling – same number of electrons as lattice sites. (Don’t forget about spin!) Describe which states in the band structure are filled, and which are empty. You should find “Dirac points,” where the band structure looks as shown in Fig. 4b – the band structure looks like this for any direction in \( k \) that passes through the Dirac point.

Where are the Dirac points in the Brillouin zone? How many distinct Dirac points are there? (Be careful – counting the number of Dirac points is a bit subtle!)
Fig. 3

$r = na$

Fig. 4a

unit cell with points $(\vec{R}, 1)$ and $(\vec{R}, 2)$

Fig. 4b.

(empty states)

(Dirac point)