Physics 7440 Problem Set 5
(Spring 2008, M. Hermele)

1. Ashcroft & Mermin 5.2
2. A+M 5.4
3. A+M 9.1
4. A+M 9.3
Consider a 1d chain, with a single tight-binding orbital on each site $r = n\alpha$, ($n$ is an integer, $\alpha$ is the lattice spacing).
Let $C_r^\dagger$ create an electron at site $r$ with spin $\sigma$.

Suppose that, as shown above, on "even" bonds the hopping matrix element is $t$, while on "odd" bonds it's $t'$.

(a) Write down the tight-binding Hamiltonian in terms of $C_r^\dagger$.

(b) Suppose we add electrons to the system until the number of electrons is the same as the number of lattice sites. This is called "half-filling," since $\langle C_r C_r \rangle = 1$, while its maximum value is 2.

Solve for the tight-binding band structure in the case $t = t'$, using the smallest possible unit cell.

Plot $E_n(k)$ 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 using the smallest possible unit cell. Again, indicate which states are occupied by electrons (assuming half-filling, as before).

(d) What is the physical distinction between the ground states found above when (1) $t = t'$ and (2) $t \neq t'$?
6. Tight-binding band structure of graphene

Graphene can be modeled by a single tight-binding orbital on each site of the honeycomb lattice. If we call the honeycomb sites \( \mathbf{R}_i \) and let \( c_{\mathbf{R}_i}^\dagger \) create an electron at \( \mathbf{R}_i \) with spin \( \sigma \), the tight-binding Hamiltonian is:

\[
H_{TB} = -t \sum_{\langle \mathbf{R}_{i',i} \rangle} \left[ c_{\mathbf{R}_i}^\dagger \cdot c_{\mathbf{R}_{i'}\sigma} + c_{\mathbf{R}_{i'}\sigma}^\dagger \cdot c_{\mathbf{R}_i} \right]
\]

The sum is over nearest-neighbor bonds.

You may find it convenient to label the sites by \((\mathbf{R}, i)\), where \(i = 1, 2\) labels the two-site basis as shown.

Also, \( \mathbf{R}_i = \mathbf{R}_0 + \mathbf{a}_i \), where
\[
\mathbf{a}_1 = \frac{\hat{x}}{2} + \frac{\sqrt{3}}{2} \hat{y}
\]
\[
\mathbf{a}_2 = \mathbf{a}_1 + \mathbf{a}_2 = \mathbf{a}_1 + \frac{\sqrt{3}}{2} \mathbf{a}_2
\]
9) Write down the primitive vectors for the reciprocal lattice, and draw the corresponding Brillouin zone.

(b) Solve for the tight-binding band structure. You should find two bands.

(c) Plot the band structure along the line $k_y = 0$.

(d) Suppose, as is the case in graphene, that we are at half-filling — same number of electrons as lattice sites. Describe which states in the band structure are filled, and which are empty.

You should find "Dirac points," when the band structure looks like:

Where are the Dirac points in the Brillouin zone?

How many distinct Dirac points are there?
(c) Consider the velocity \( V_k = \frac{1}{\hbar} \frac{\partial \varepsilon_n(k)}{\partial k} \) near the Dirac points. (You can focus on the band corresponding to the empty states.)

If \( \vec{k}_0 \) is the location of a Dirac point, calculate \( V_{\vec{k}} \) for \( \vec{k} = \vec{q} + \vec{k}_0 \), keeping only lowest-order terms in \( \vec{q} \).

Express your answer in terms of \( \vec{t} \) and \( \alpha \).

Is \( |V_{\vec{k}}| \) the same in all directions moving away from the Dirac point?