1. **Carbon Nanotube Structure**: Derive the expressions for the unit vectors of graphene (unrolled nanotube) $\mathbf{a}_1, \mathbf{a}_2$, in terms of the Cartesian unit vectors $\mathbf{x}, \mathbf{y}$. (a) Using trigonometry, show your calculations for the numerical factors $a$ and $b$ (e.g. $\frac{1}{2}$ or whatever) in terms of the length of the carbon-carbon bond length, $a_o$. (b) sketch and indicate the unit cell in real space, which is the parallelogram spanned by $\mathbf{a}_1$, and $\mathbf{a}_2$. Hint, consider the figures below.

\[
\begin{align*}
\mathbf{a}_1 &= a\mathbf{x} + b\mathbf{y} \\
\mathbf{a}_2 &= a\mathbf{x} - b\mathbf{y}
\end{align*}
\]

\[
\begin{align*}
\mathbf{a}_1 &= a\mathbf{x} + b\mathbf{y} = \frac{3}{2} a_o \hat{x} + \frac{\sqrt{3}}{2} a_o \hat{y} \\
\mathbf{a}_2 &= a\mathbf{x} - b\mathbf{y} = \frac{3}{2} a_o \hat{x} - \frac{\sqrt{3}}{2} a_o \hat{y}
\end{align*}
\]

2. **Carbon Nanotube Dispersion**: Consider the dispersion relation for graphene:

\[
W(k_x, k_y) = \pm \gamma_0 [1 + 4\cos(\sqrt{3}k_x a_0/2) \cos(k_y a_0/2) + 4\cos^2(k_y a_0/2)]^{1/2},
\]

following the notation in Waser, where $a = \sqrt{3}a_o$ is the length of the unit vector $\mathbf{a}_i$, and $a_o$ is the length of the carbon-carbon bond (0.142 nm). Note that this “$a$” differs from the convention used above in question 1. (a) Find the six Fermi level conduction points in $k$-space (which are the corners of the hexagonal Brillouin zone below) by solving for the $k$ values where $W(k_x, k_y) = 0$. (b) On the hexagonal Brillouin zone, sketch and label the coordinates of these 6 points in terms of $a$, or $a_o$.

Hint: in the dispersion relation first let $k_x = 0$ and solve for the corner points along $k_y$; and then let $\sqrt{3}k_x a_0/2 = \pi$, and get the corners with $k_x \neq 0$. This approach makes it easier to factor the dispersion terms under the root as a perfect square. Then take the square root and solve for $k_{x,y}$.

Let $\sqrt{3}k_x a_0/2 = 0$: $W(k_x, k_y) = 0 = \pm \gamma_0 [1 + 2\cos(k_y a_0/2)]$, which gives $k_y a_0/2 = 2\pi/3$

Let $\sqrt{3}k_x a_0/2 = \pi$: $W(k_x, k_y) = 0 = \pm \gamma_0 [1 - 2\cos(k_y a_0/2)]$, which gives $k_y a_0/2 = \pi/3$
3. **Carbon Nanotube Metallic condition:** Show that the condition for metallic conductivity of chiral nanotubes: \(2n_1 + n_2 = 3q\), where \(q\) is an integer, can be obtained by substituting the \(\mathbf{k}\) vector of one of the corner points of the Brillouin zone into the periodic boundary condition: \(\mathbf{C}_h \cdot \mathbf{k} = 2\pi m\), where \(\mathbf{C}_h = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2\) is the chiral vector, and \(m\) is an integer. (Hint: use vector coordinates with respect to \(x\) and \(y\), and a zone boundary point that has both \(x\) and \(y\) components).

\[
\begin{align*}
\vec{c} &= m\vec{a}_1 + n\vec{a}_2 = \hat{x}a(m + n) + \hat{y}b(m - n) \\
\vec{k} &= \hat{x}k_x + \hat{y}k_y \\
\vec{k} \cdot \vec{c} &= k_x a(m + n) + k_y b(m - n) = 2\pi q
\end{align*}
\]

For metallic conduction, if \(k_x a = 0\), then \(k_y b = 2\pi/3\)

\[
\frac{2\pi}{3} b (m - n) = 2\pi q \quad \Rightarrow \quad \frac{m - n}{3} = q : \text{integer}
\]

If \(k_x a = \pi\), then \(k_y b = \pi/3\), and we get:

\[
\pi (m + n) + \pi/3 (m - n) = 2\pi q, \quad \text{which gives} \quad 2n_1 + n_2 = 3q
\]

Homework assignments will appear on the web at:
http://www.ece.udel.edu/~kolodzey/courses/eleg667_016f05.html

Note: On each submission, give your name, due date, assignment number and course number.