ELECTRONIC PROPERTIES OF GRAPHENE NANORIBBONS

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My task was to write a FORTRAN Program to determine the electronic band structure of a graphene nanoribbon.

The program should be able to handle a nanoribbon of different widths.

The program should be able to handle both arrangements of nanoribbons: armchair and zigzag.
A graphene nanoribbon is a long strip of carbon atoms laid out with a narrow width compared to its length. It can be laid out in two ways:

ZIGZAG

ARMCHAIR
The electronic band structure is the ranges of energy an electron can have in the nanoribbon. The bands above zero are the conduction bands and the bands below zero are the valence bands.
Lay out a unit cell of the ribbon and the cells on each side. Determine the position of each atom relative to a particular atom.

Determine the distance between each atom of the unit cell and all other atoms including those unit cells on each side of the initial unit cell.

If the distance is equal to the bond length, a nearest neighbor, add to the Hamiltonian Matrix a value of $t$, $te^{ika}$, or $te^{-ika}$, the hopping energy, to the array cell for that pair of atoms.
Once the Hamiltonian matrix is populated, use a diagonization function to determine the eigenvalues.

Repeat many times for different values of ka. ka should vary from $-\pi$ to $\pi$.

Graph the eigenvalues against ka.
An interesting pattern appeared with the armchair arrangement: Every third graph had no band gap at $ka = 0$. This arises from a symmetry where the two edges of the ribbon are mirror images. This means armchair ribbons are semiconductors along the length of the ribbon.
8 atom unit cell

10 atom unit cell

12 atom unit cell
Zigzag shows no change in pattern other than additional bands by increasing the width of the ribbon.

There is no band gap for the edge electrons where $ka = -\pi$ and $\pi$.

This means zigzag ribbons act like a metal.
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