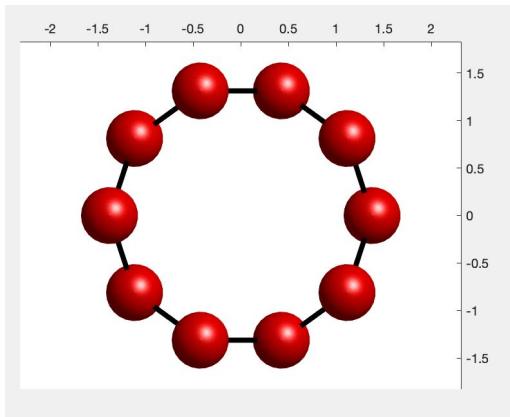


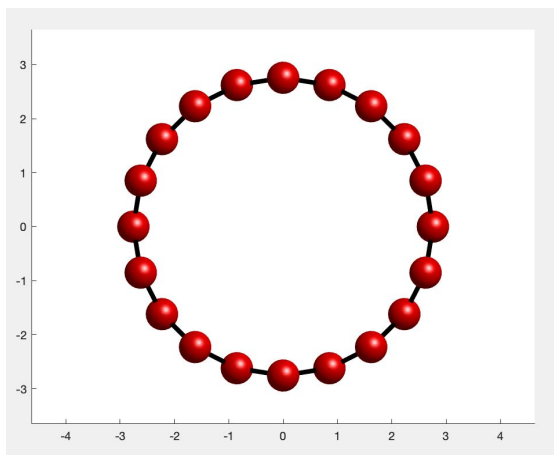
Alex Klein Project C Application

You want to encapsulate a drug within a nanotube. The drug can be approximated as a sphere of radius 4 angstroms. The carbon-carbon bond length is 1.42 angstroms. What is the smallest zig-zag nanotube that could possibly be expected to encapsulate the drug? What is the smallest armchair nanotube that could possibly encapsulate the drug? Provide images and data for each case from your code and explain your result.

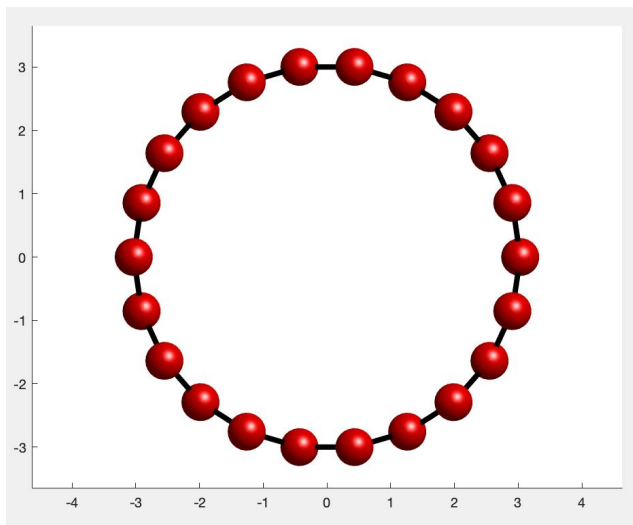
A zig-zag carbon nanotube is modeled by the function `nanotube(n,m,len)` when $m=0$. Any value of `len` can be chosen because we are only concerned with the radius of 4 angstroms = diameter of 8 angstroms, but we will choose `len = 2` to easily view the tube from its end. However, because each carbon-carbon bond length is 1.42 angstroms, we divide $8/1.42$ to find that we are looking for a tube of 5.634 units in our simulation. We choose the arbitrary value $n=5$ to start...



...and see that it has a diameter of 3 units and is clearly not large enough. Now that we have a baseline, we run `nanotube(10,0,2)` to return the following output:

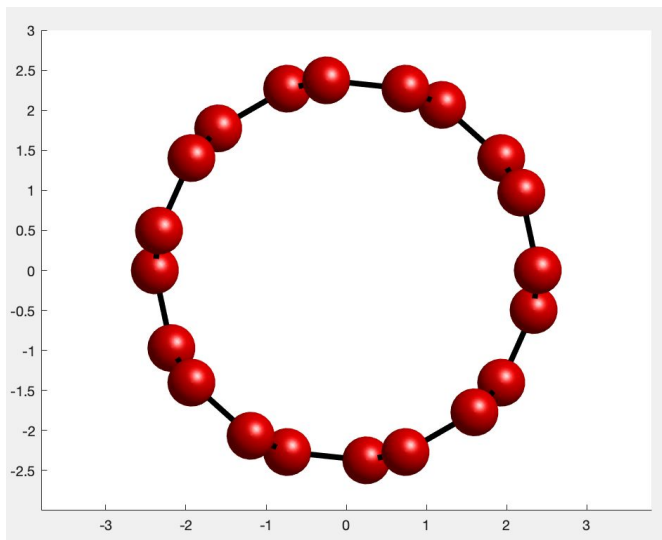


This tube has a diameter of 5.48 units (based on the coordinate grid) and is too small. Now, we will test the next size zig-zag tube up: `nanotube(11,0,2)`.

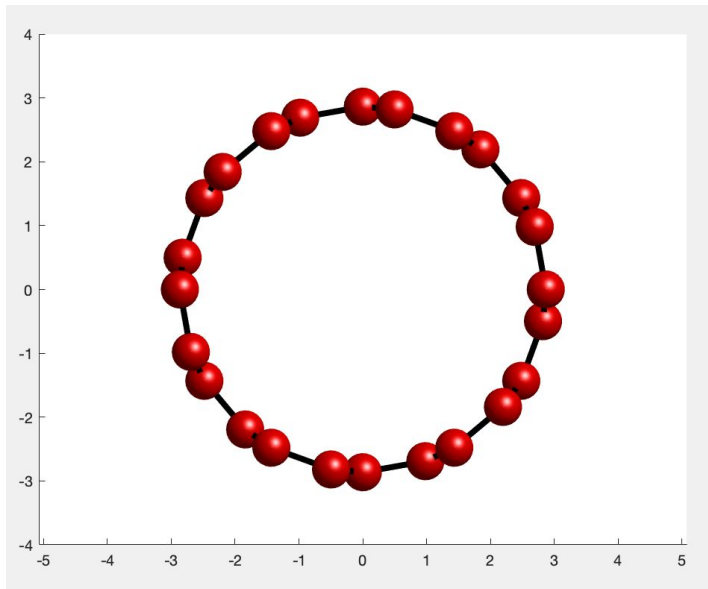


This tube has a diameter of 6.02 units (based on the coordinate grid) and will fit the drug with radius 4 angstroms.

An armchair tube is where $n=m$. We set the `len = 2` again for simplicity and try `nanotube(5,5,2)`:



This tube has a diameter of 5.73 units (based on the coordinate grid) and is too small. Now, we will test the next size armchair tube up: `nanotube(6,6,2)`.



This tube has a diameter of 5.73 units (based on the coordinate grid) and will fit the drug with radius 4 angstroms.

In conclusion:

- The smallest zig-zag nanotube that could encapsulate the drug is $n = 11$, $m = 0$
- The smallest armchair nanotube that could encapsulate the drug is $n = 6$, $m = 6$