Verification of the Validity of the CNTBands Tool

According to experimental data the band gap of semiconducting nanotube is inversely proportional to its radius. The simple analytical model also explained in solution for homework Problem 3 indicates that the prefactor ***V*** in this dependence is the absolute value of the nearest neighbor tight-binding element in the pi-orbital approximation

$$E_{g}=\frac{V}{R}$$

Here CNT radius ***R*** is measured in the units of carbon-carbon bond length. If ***R*** is expressed in nanometers,

$$E_{g}=0.142\frac{V}{R}$$

The plot below, which collects data from *CNTBands* pi-orbital tight-binding simulations (dark-blue circles) demonstrates that this is indeed the case. The solid red line is the inverse dependence given by the equation above.