Lab Assignment 8 (2022)
PH-566

1. According to Lanczos algorithm for nonlinear lattice, the Green function matrix element is defined as

$$G_{ii}(z) = \cfrac{b_1^2}{z - a_1 - \cfrac{b_2^2}{z - a_2 - \cfrac{b_3^2}{z - a_3 - \cfrac{b_4^2}{\ddots \cfrac{}{z - a_N - b_{N+1}^2 T(z)}}}}}$$

where a_i's, b_i's are real numbers and z is a complex variable (z=E+iδ; E is the energy). T(z), which serves the purpose of terminating the continued fraction, is defined as

$$T(z) = \frac{z - a_N - \sqrt{(z - a_N)^2 - 4b_{N+1}^2}}{2b_{N+1}^2}$$

Using do-loop statement, write a code to calculate the above-mentioned Green function in the energy range E= (-10,10) in steps of 0.01 (don't worry about units) taking the imaginary part of E, i.e. δ = 0.001.

Take the values of a_i and b_i from the supplied data file named "data.txt" (They are arranged in a given row as i, a(i), b(i+1); highest i represents termination of the continued fraction (i.e. $(i)_{max}=N$). Also, consider b(1)=1.0)

Hence, calculate the basis-projected density of states $n_i(E)$, defined as

$$n_i(E) = -\frac{1}{\pi}\Im m[G_{ii}(z)]$$

Print *E* vs. *n(E)* in a data file named "DOS.dat". Hence, plot this data in gnuplot.