

A study on the properties of fractal electronic quantum systems

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Introduction

The main objective of this project is to investigate the properties of fractal (Sierpinski triangles) electronic quantum systems (EQS), specifically when defects are introduced, by means of Recursive Green's Functions methods (RGF).

The electronic structure of such systems can be described using a simple tight-binding Hamiltonian

$$H = \sum_i \epsilon_i c_i^\dagger c_i - \sum_{\langle i,j \rangle} t_{ij} (c_i^\dagger c_j + H.c), \quad (1)$$

where the on-site energy is denoted by ϵ , t_{ij} is the hopping term between sites i and j , $H.c$ is the Hermitian conjugate and c_i^\dagger and c_j are the creation and annihilation operators.

Three types of the Sierpinski lattices were investigated (shown in the Fig. 1).

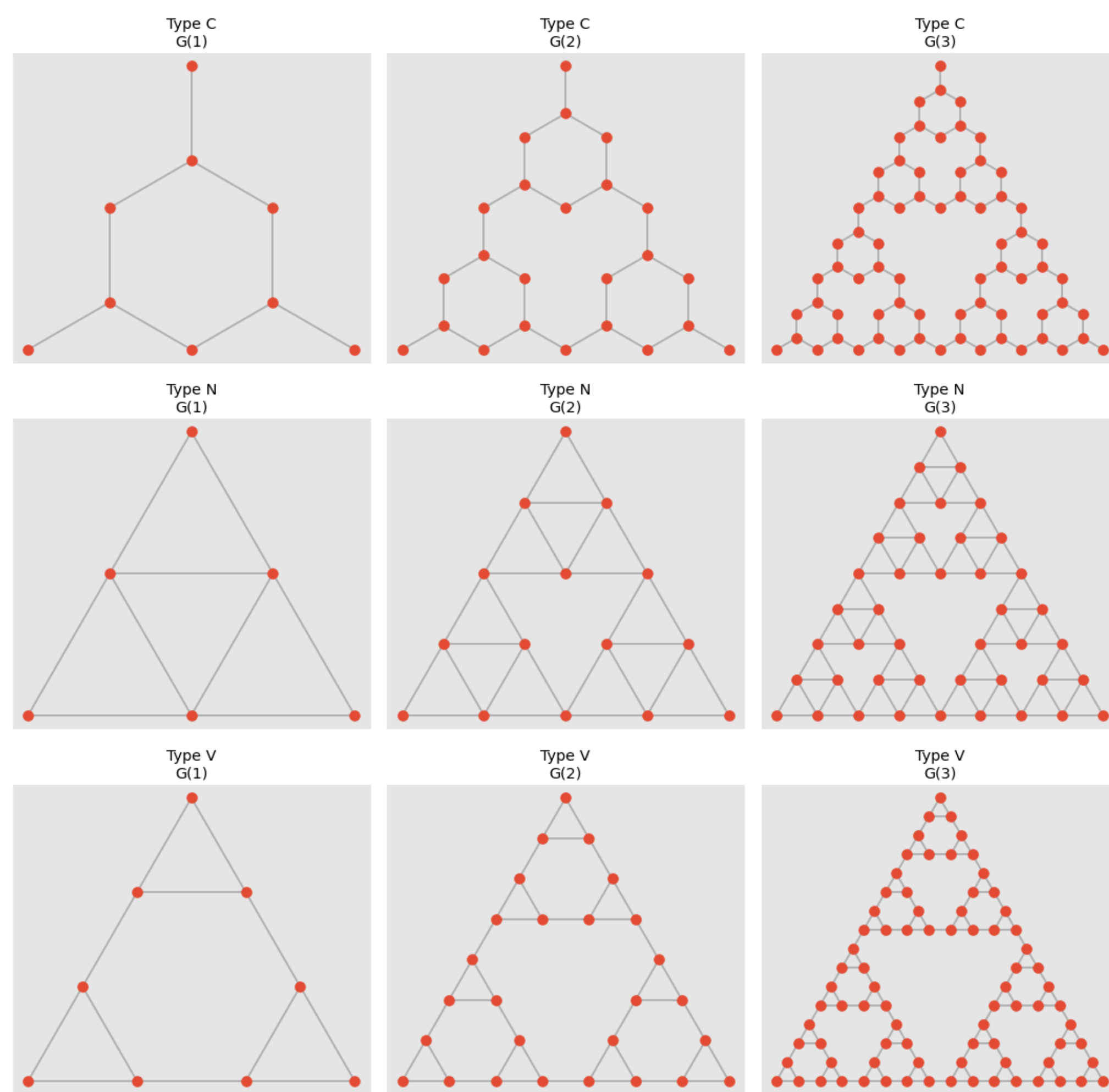


Figure 1: The first three iterations of the three variations of the Sierpinski triangle fractal lattices that were studied. The type N lattice was obtained by removing the centre points of each unit triangle in the type C lattice. The type V lattice was obtained by separating the vertices of each unit triangle in the type N lattice such that the unit triangles do not share vertices.

Recursive Green's Function

To use the RGF it is necessary to first divide the lattice into cells such that each cell neighbours only the previous and next cell. The process is then based on iteratively adding the cells to the system and using the Dyson equation to find the Green's function of composite system.

Consider two systems: the 'clean'/initial system defined by $H = H_0$, $g = (EI - H_0)^{-1}$ and the perturbed system defined by $H = H_0 + V$, $G = [EI - (H_0 + V)]^{-1}$. Then, the Dyson equation is given by

$$G = g + gVG. \quad (2)$$

Results

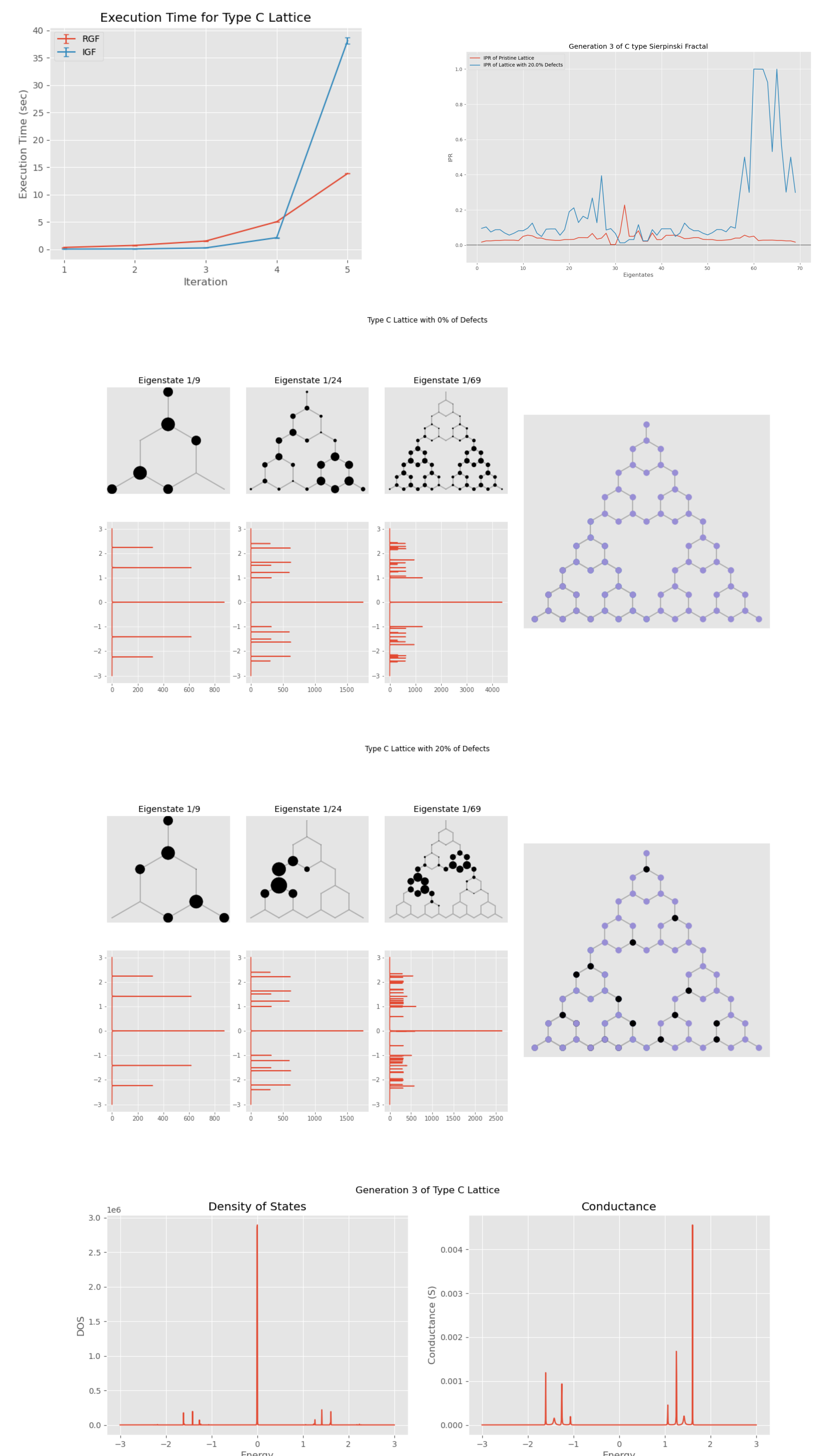
- The brute force method was faster for simpler systems (iteration 4 or less), but for lattice of iteration 5 or higher it is significantly slower.
- The addition of defects to the lattice cause the eigenstates to be more localised as can be seen by higher IPR for the majority of the states.

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Results Cont.

- The defects were added by largely increasing the on-site energy of randomly selected sites. This type of defect corresponds to replacing the atom with an atom of a different element.
- The conductance was calculated and plotted together with the DOS. Both plots have peaks for similar values of energy except the 0 energy for which the DOS has the greatest value while conductance is null.



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References

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