Guide to Run Our Codes

Computational Physics, PH-354

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This document provides a guide for running the provided codes.

1. I have shared 6 different `.py` files in the folder named `source code`.

2. Start with `2_band_model.py` and `4_band_model.py`, which show the band structures for monolayer Phosphorene.

3. Then, open `(1)_zPNR.py`, which contains all the calculations for the zig-zag nanoribbon. Simply run the file, and it will display all the graphs one by one.

4. Next, open `(2)_aPNR.py`, which contains all the calculations for the armchair nanoribbon. Again, you can run the file to see the graphs. If you want to visualize the plots for the 50-aPNR at different hopping values, you can edit line 334, changing 10 to 50, and adjust the t_2 hopping parameter accordingly.

5. Finally, there are two files to plot the transmission of electrons in different systems:

- `Transmission_10-zPNR.py`: This file calculates the transmission for 10-zPNR as both the device and leads.
- `Transmission_Square_Lattice.py`: This file calculates the transmission for a square lattice as both the device and leads.

Note: These transmission files may take some time to run even after the parallelisation of Energy grid in 8 processors, especially the 10-zPNR device. While running this file, the output will display progress in the following format:

The first column shows the iteration step number, the second column shows the energy, and the third column shows the convergence parameter, which is the absolute sum of the matrix elements of the difference between two consecutive matrices in Dyson's equation.