Band Structure and Topological Invariance Calculations of Materials Utilizing DFT Simulations on Quantum Espresso

By

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Overview

ICTP:PWF internships taught students about various subjects from the field of physics and mathematics. As a part of this internship our purpose was to learn the basics of band structure and phonon dispersion curve of materials, to learn calculating them using density functional theory simulations with the utilization of the software Quantum Espresso, and also to plot the data. Furthermore, we explored the calculation of quantum topological invariance of these materials from the simulation results by using python codes. Additionally, we have learned linear algebra and Fourier transformation.

Objectives

- To study quantum harmonic oscillators to understand, band formations
- To study linear algebra and Fourier transform for better understanding of the band formations
- To learn DFT simulations using Quantum Espresso
- To find the Z2 invariance of the material using python package

Introduction

Every material has inherent properties which can be observed and calculated via the Density Functional Theory (DFT) simulations. These simulations are solely based on quantum mechanics and can be described by the Schrodinger's Equation [2,3]. While the basis of DFT can be described by the Schrodinger's Equation, the DFT calculations are not feasible utilizing the Schrodinger's Equation [2]. Even the term DFT is not directly derived from Schrodinger's theory. Rather it came from the Kohn-Sham equation [1]. Many scientists have worked on the simplification process of the Schrodinger's Equation, but eventually the Kohn-Sham approach was accepted by all [3]. Kohn-Sham approach simplifies the electronic interactions by simplifying electron numbers as electron densities which helps us to avoid the many body problem arising from multi electron systems. On the other hand, it also ignores nucleus-nucleus interactions for simplification of the calculations [3]. The Kohn- Sham equation is the following-

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{eff}(r)\right]\psi_i(r) = \varepsilon_i\psi_i(r) \tag{1}$$

Here,

$$V_{eff}(r) = V_{\text{ext}} + V_H + V_{xc} \tag{2}$$

All the potential terms associated with Kohn-Sham equation are summed as the effective potential V_{eff} as a function of r which is the radius of the electron density cloud. The effective potential depends on the potential generated by the interactive forces between the particles. V_{ext} is the external potential by which we get the interaction between electron and nucleus. This potential is very strong near the nucleus- electrons are tightly bound in core states, and their wavefunctions oscillate rapidly in that region. A pseudopotential simplifies DFT calculations by replacing the strong nuclear potential with a smooth, weaker one that eliminates core electrons while preserving the correct behavior of valence electrons outside the core region [4,5]. Some of the most common pseudopotentials are UPF (ultrasoft), PAW (Plane Augmented Wave) etc. The potential V_{H} defines the Coulombic interaction between electrons, which develops an electrostatic force. Finally, V_{xc} is the most significant contributor of them all, although the numerical value is very small compared to the other parts of effective potential but the impact on the electronic properties, especially bandgap is very significant [6]. XC represents Exchange-Correlation, where the exchange energy comes from Pauli's exclusion principle, which defines two electrons with the same spin cannot stay in the same point in space. On the other hand, correlation describes the electron motion correlation due to mutual repulsion.

In this study, our main purpose was to understand the basics of simple quantum mechanics to explain the band and phonon dispersion structure formation. Also, some mathematical studies on the topics Linear Algebra and Fourier Transform were completed for better understanding of the derivations of DFT theories. Further, the complex calculations involved in DFT simulations were explored utilizing simulation software, Quantum Espresso [7]. Utilizing this software, we can optimize the geometry of a structure and find the structural parameters of the structure. From the optimized structure the calculation of the self-consistent field/ non self-consistent field of the structure is possible, and from these calculations we can find the band structure of the material, also the density of states and phonon dispersion calculation is possible [7,8]. Furthermore, utilization of PWTK makes the work swift and neat, and the utilization of Wannier90 tools can help to get the Hamiltonian and study the topological invariance of the structure [8]. Finally, the utilization of python code packages (z2pack) can calculate Z2 invariance of the structure.

Results and Discussion

In this section I will present my learning and contribution throughout the internship period:

At the initial stage, we learned the basics of Quantum Mechanics (QHM), Linear Algebra, and Fourier Transformation. We discussed and solved several simple problems to strengthen our understanding. Additionally, we started preparing a logbook to document the entire internship process. My contribution to the logbook included adding the section on Linear Algebra, with relevant notes and examples. (Snapshots from the logbook are provided below.)

5.4 System of Linear Equations

5.4.1 Rewriting in Matrix Form

Sometimes it's better to write the coefficients on the right.

The vector **b** is just a linear combination of the column vectors of matrix A.

Solving a system of linear equations means finding the coefficients of the linear combination, here x and y.

Imagine you have vectors $\mathbf{e}_1$ and $\mathbf{e}_2$.

Multiplying a vector **x** by a matrix A from the left gives us a new vector **b**. Another way of saying this is that we take a linear combination of the column vectors of A to get **b**, and the scalar multipliers of that linear combination are the components of **x**.

If we have

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix},$$

then

$$A\mathbf{x} = \mathbf{b}.$$

5.4.2 Methods to Solve System of Linear Equations Using Matrices

a) Gaussian Elimination
b) Gauss Jordan
c) Determinant Method

5.5 Eigenvalues and Eigenvectors

If

$$A\mathbf{x} = \lambda\mathbf{x},$$

where λ is a scalar, then

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$$A\mathbf{x} = \lambda \mathbf{x},$$

where λ is a scalar, then

- λ is the eigenvalue,
- $\mathbf{x}$ is the eigenvector.

We ask the question: what are the set of vectors that get scaled by λ as a result of matrix multiplication?

$$(A - \lambda I)\mathbf{x} = 0$$

So, $(A - \lambda I)$ is a singular matrix if $\mathbf{x}$ is not null. The determinant of a singular matrix is zero:

$$\det(A - \lambda I) = 0.$$

Here, I is the identity matrix.

5.5.1 Example

Let

$$A = \begin{bmatrix} -1 & -3 \\ 1 & -1 \end{bmatrix}.$$

We compute:

$$\det(A - \lambda I) = 0$$

$$\det \begin{bmatrix} -1-\lambda & -3 \\ 1 & -1-\lambda \end{bmatrix} = 0$$

$$\Rightarrow (-1-\lambda)(-1-\lambda) - (-3)(1) = 0$$

$$\Rightarrow (\lambda + 1)^2 + 3 = 0$$

$$\lambda^2 + 2\lambda + 4 = 0$$

$$\lambda = -1 \pm i\sqrt{3}.$$

(Replace with the example in your notes if needed. In the original text, it simplifies to $\lambda^2 + 4\lambda + 3 = 0$, yielding $\lambda = -3, -1$.)

5.5.2 Normalization

Since $\mathbf{x}$ is arbitrary, we can choose a particular form for the eigenvector.

For normalization, we define

$$\mathbf{u} = \frac{\mathbf{x}}{\|\mathbf{x}\|}.$$

Thus, eigenvectors can be normalized to unit length.

5.5.3 Diagonalization

If A is diagonalizable, then

$$A = U \Lambda U^{-1},$$

where U is the matrix of eigenvectors and Λ is the diagonal matrix of eigenvalues.

Moving forward, we learned to perform basic simulations in Quantum ESPRESSO, including vc-relax, scf, nscf, band, and DOS calculations. After mastering these fundamental techniques, we progressed to using PWTK, conducted Wannierization, and later calculated topological invariants using Python scripts.

Following the learning phase, we began working on a 2D material to investigate its properties. Every member of our group is actively contributing to this research. My personal contributions include preparing the vc-relax, scf, and nscf input files for this material, as well as creating a GitHub repository to organize and share our codes.

GitHub- https://github.com/DilwarAlvee/ICTP-Project.git (as our work is still in progress the git is private for the time being). My vc-relax code for our material is shared below-

```
&CONTROL
    calculation = 'vc-relax',
    prefix = 'wte2',
    outdir = './',
    pseudo_dir = '\pseudo',
    verbosity = 'high',
/

&SYSTEM
    ibrav = 0,
    nat = 6,
    ntyp = 2,
    ecutwfc = 80.0,
    ecutrho = 640.0,
    occupations = 'smearing',
    smearing = 'gaussian',
    degauss = 0.005,
    assume_isolated = '2D',
/

&ELECTRONS
    conv_thr = 1.0d-8,
    mixing_beta = 0.3,
/

&IONS
    ion_dynamics = 'bfgs',
/

&CELL
    cell_dynamics = 'bfgs',
    press_conv_thr = 0.5,
    cell_dofree = '2Dxy',
/

ATOMIC_SPECIES
W   183.84  W.UPF
Te  127.60  Te.UPF
```

```
CELL_PARAMETERS (angstrom)
3.50   0.00   0.00
0.00   6.33   0.00
0.00   0.00  24.22

ATOMIC_POSITIONS (crystal)
W   0.00000  2.8837   12.2139
W   1.7502   0.6368   12.0057
Te  0.00000  1.2517   10.0013
Te  1.7502   4.4718   10.6254
Te  1.7502   2.2692   14.2182
Te  0.00000  5.3766   13.5942

K_POINTS (automatic)
8 4 1 0 0 0
```

Conclusion

Over the course, all objectives were successfully achieved. We learned the fundamentals of Quantum Mechanics (QHM), Linear Algebra, and Fourier Transformations. Subsequently, we explored Density Functional Theory (DFT) calculations using Quantum ESPRESSO. Initially, we performed simulations on silicon, and later began experimenting with our own material systems.

References

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Approval

The internship report titled **“Band Structure and Topological Invariance Calculations of Materials Utilizing DFT Simulations on Quantum Espresso”** submitted by **Mohammad Dilwar Ali Alvee**, a participant of the ICTP PWF: Physics for Bangladesh Online Summer Internship, has been found satisfactory in partial fulfillment of the requirements of the internship program.

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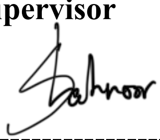
Supervisor



5. 11. 2025

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