Application of X-Ray Diffraction on the Proof of Topological Edge States of Monolayer Graphene

ABSTRACT

This research aims to decipher whether monolayer graphene exhibits topological properties, focusing on the computational side. The edge states of topological insulators can be difficult to predict using traditional methods, so we used the principles of the Schrodinger Equation, Bloch's Function, the Linear Combinations of Atomic Orbitals (LCAO), and Tight Binding Tool Kit (TBTK) to calculate the electronic band structure for graphene [4]. We first derived the periodic boundary condition for the Graphene lattice, which was necessary for the computation of the reciprocal lattice space of the crystal using x-ray diffraction. With this information, we could easily solve for the crystal momentum vector k, which gave us information on the momentum space of electrons in the lattice. Normalizing this function with orbital overlapping function, we obtained the tight-binding Hamiltonian for Graphene, to which we converted to momentum space and graphed the electronic band structure by utilizing the TBTK software. By analyzing the results, we concluded that monolayer graphene is a possible topological insulator, since the energy bands intersected at the Dirac points (or the edges), while eliciting a wider band gap at its bulk.

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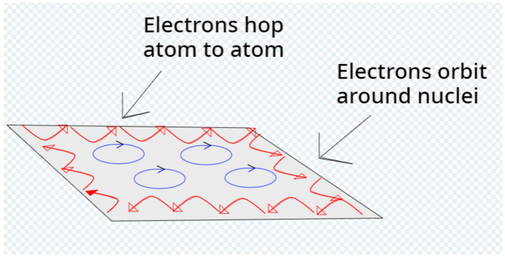
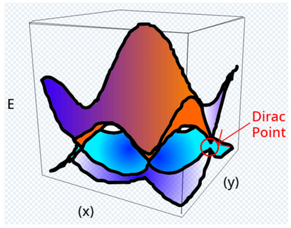
01. Introduction

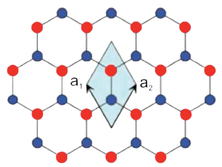




Band energies of Graphene's Bravais lattice mapped in two dimensions.

Graphene holds interesting electrical properties due to the fact that bilayer graphene is a topological insulator. A topological insulator is a material which exhibits conductivity on its edges of the surface but is an insulator in most of its mass. For instance, a 3D topological insulator will show conductivity on its faces while a 2D one has so on its edges. A crude simplification of the idea is the model up above. While electrons in the center orbit around their nuclei as usual, electrons on the edge have nowhere to go, so they bounce around the edges of the material.

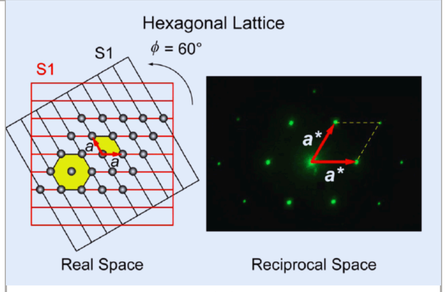
One way to explain this is by deeply analyzing the periodicity of the potential energy of different lattice structures within the crystal, which reveals valuable information about the energy and momentum of the electrons, and in turn, the band structure. Furthermore, analysis of the band structure can yield critical information on the electrical properties of the lattice, such as conductivity. In the case of Graphene, we only need to quantify our calculations to two dimensions, since the Carbon allotrope is only a single atom thick.



(1) Structure of Graphene: a hexagonal lattice. Blue: sublattice A. Red: sublattice B. a_1 and a_2: lattice vectors

02. Objective

Our goal is to uncover information about the LCAO, Bloch function, and periodic boundary condition of Graphene, in order to synthesis the Tight-Binding Hamiltonian for Graphene, a matrix containing all energy eigenstates as a function of the crystal momentum space. Applied to the wave function and using TBTK for graphing, this will show us the intersection of all band structures at any point in the lattice space.



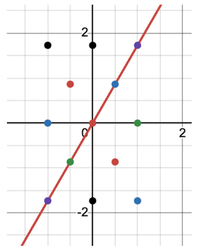
(2)

By using single crystal x-ray diffraction, we can transform the real space hexagonal lattice to reciprocal space, as in the case of graphene. a is the reciprocal lattice vector.*

03. Methodology

The process involved calculating the periodic boundary condition for Graphene's Bravais lattice, determining the reciprocal lattice using a Discrete Fourier Transform, and applying it to the Hamiltonian operator in the tight-binding model. Crystal Field Theory was used to address orbital overlap, equating and normalizing LCAO and Bloch functions. With the new equation and wave functions for orbital types, we were able to calculate each element of the operator. Calculations for overlapping orbitals were made. Graphene's 4 types (S, P(x), P(y), P(z)) result in 16 orbital interactions between atoms, leading to a 4x4 matrix. With self-interactions, the Tight-Binding Hamiltonian becomes an 8x8 matrix with 64 elements.

Bravais lattice boundary condition



$$V(x,y) = V\left(x + \frac{N_x a}{2}, y + \frac{\sqrt{3}}{2}\left(x + \frac{N_x a}{2} + 2N_y a\right)\right) \quad V(x,y) = V\left(x + \frac{2N_x \pi}{a}, y + \frac{2}{\sqrt{3}}\left(\frac{N_x \pi}{a} + \frac{2N_y \pi}{a}\right)\right)$$

This Hamiltonian was crucial for us to understand the band structure in the Brillouin zone at the high symmetry points(Γ, K, and M). By inserting parameters into the tight-biding Hamiltonian and using TBTK to graph it, we obtained the following band structure. In graphene, t = 3 eV.

Normalization of LCAO with the Bloch Function: $\psi_{nk}(x) = \frac{1}{\sqrt{N}} \sum_R e^{ik\cdot R} \phi_{nR}(x)$

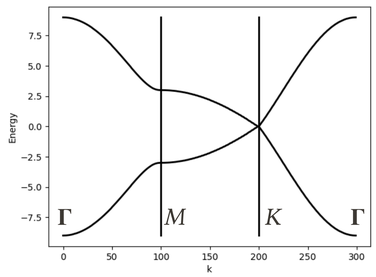
Reciprocal Transform

How to theoretically use X-ray diffraction to find the reciprocal lattice.

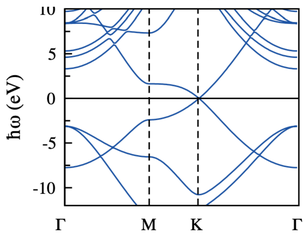
Tight-binding model in real space: $H = -t \sum_{i\delta} c^{\dagger}_{i,A} c_{i+\delta,B} + H.c.$

Tight-binding model in reciprocal space: $H = -t \sum_{k} c^{\dagger}_{k,A} c_{k,B} \left(e^{ik\cdot r^{(0)}_{AB}} + e^{ik\cdot r^{(1)}_{AB}} + e^{ik\cdot r^{(2)}_{AB}}\right) + H.c.$

04. Results



Our band structure graph generated using TBTK and C++



(3)

05. Analysis

By comparing our generated band structure to the band structure obtained by other researchers through experiments, it's evident that the intersections at K are almost identical, while the energy bands diverge at Γ. This matches the band structure obtained by other researchers' experiments. The intersection suggests that electrons can hop to a higher energy band, leading to conductivity in the Brillouin zone at edge K. The split at Γ suggests that electrons won't be able to hop over because it is an insulator at the bulk. Therefore, monolayer graphene has the potential to become a topological insulator.

06. Conclusion

- *We first obtained the reciprocal lattice and the boundary conditions for the hexagonal lattice of graphene.*
- *By implementing the Schrodinger's equation, and normilizing LCAO with Bloch's function, we were able to unlock the energy eigenstates of electrons and thus find the tight-binding Hamiltonian to describe the band structure.*
- *In closure, we have shown how single X-ray diffraction can play a crucial role in proving the topological edge states of monolayer Graphene, since the reciprocal lattice contributes to the wave function, and therefore the calculation of the electronic band structure.*
- *By implementing similar steps of process, we are also able to predict the topological properties of more complex substances.*
- *TIs have surface states that are robust against scattering and impurities, making them ideal candidates for stable qubits in quantum computers. They have the potential to revolutionize various fields of technology, leading to more efficient, stable, and innovative devices.*

Future Directions

1. *Calculate the Berry phase and Berry curvature*
2. *Topological Invariant; The Chern Number*
3. *Using the tight-binding model, predict the electrical properties of future topological insulators.*

References

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