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Computational Investigation of Electronic Band Structure in Graphene Using Tight-binding Approximation

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Abstract

Graphene is a two-dimensional allotrope of carbon arranged in a honeycomb lattice, representing a fundamental material in condensed matter physics due to its exceptional electronic properties. The electronic band structure of graphene is investigated computationally in this research. Analyzing the source of graphene's semimetallic properties and describing its low-energy electronic dispersion are the primary aims of the research. The methodology is based on constructing graphene's reciprocal lattice and computing the tight-binding Hamiltonian over a discretized Brillouin zone with a k-space grid resolution of 200 × 200 points. Three-dimensional surface plots and two-dimensional contour maps are used to depict the resulting electronic energy dispersion calculated on a two-dimensional momentum grid. The Brillouin zone's high symmetry points where Dirac cones form and govern low-energy physics receive particular attention. The conduction and valence bands meet at discrete Dirac points with a zero band gap of 0.0 eV, confirming the semimetallic nature of graphene. The energy dispersion becomes linear near these values, following the relation E = ±ℏvF|k| in the low-energy regime (|E| < 1.0 eV), indicating that charge carriers behave like massless Dirac fermions with a Fermi velocity of vF ≈ 1.0 × 10⁶ m/s. The energy range spans approximately − 3.0 eV to + 3.0 eV with a total bandwidth of approximately 6.0 eV. The contour plot shows hexagonal symmetry compatible with the underlying graphene lattice, while the tight-binding model captures lattice effects that cause deviations from linearity away from the Dirac points. The hopping parameter t = 2.8 eV used in the simulation accurately reproduces the electronic structure. The results demonstrate that the fundamental electrical characteristics of graphene are successfully replicated by the tight-binding approximation, establishing it as a reliable computational framework for investigating two-dimensional quantum electronic systems.

INTRODUCTION

Condensed matter physics and its ability to explain the structural, electrical, magnetic, and the transport properties of materials has become an important areas in the study of modern physics. It shows how atoms and electrons act together in solid and low dimensional system. One of its major achievement is the development of the electronic pan theory which provides a way to understand the electrical behavior of conductors, semiconductor, and insulators (Ashcroft and Mermin, 1976). The arrangement of atoms in a crystalline materials, create energy bands and band gaps. The energy dispersion relation is frequently used to characterize the electrical characteristics of a crystalline solid.

$$E = E\left(k\right)$$

This establishes a reciprocal spatial relationship between electron energy and crystal momentum. Graphene is one of the materials which has gained the most attention from scientist due to its electrical and physical characteristics. A single atomic layer which is organized in an hexagonal honeycomb lattice arrangement is a graphene. Novoselov et al., (2004) separated graphene from graphite approved the assistance of stable two dimensional crystals, which sparked further research into graphene based system. It has an exceptional, electrical mobility, mechanical, strength and high thermal conductivity

(Geim and Novoselov, 2007). It's unusual electrical structure in contrast to semiconductors as a zero bank gap electronic spectrum that features Dirac points specific locations within the Brillouin zone where the conduction and valence bands overlap (Wallace, 1947). Charge carriers act as massless Dirac fermions instead of traditional electrons and it follows a linear energy momentum connection (Castro Neto et al., 2009). It's peculiar electronic phenomenon like an exceptionally high carrier mobility, anomalous quantum Hall effects are caused by this relativistic like behavior (Zhang et al., 2005; Gisynin and Sharapov, 2005). The electronic dispersion relation of graphene can be written as follows within the nearest-neighbor tight-binding approximation:

$$E(k) = \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_y a}{2}\right)\cos\left(\frac{k_x a}{2}\right) + 4\cos^2\left(\frac{k_x a}{2}\right)}$$

where t denotes the nearest-neighbor hopping parameter, while $k_x and\, k_y$ represent the reciprocal lattice wave vectors. The conduction and valence bands are represented by the positive and negative branches, respectively.

Graphene has been studied extensively, both theoretically and computationally using various methods like the density, functional theory, greens function methods, and so on. The first theoretical description of graphite electronic bands was established by Wallace in 1947, a theory that will become an essential study of the graphene electron structure. Castro Neto et al., 2009 give more total analysis of the transport, electrical and quantum mechanical characteristics of graphene. While Das Sama et al 2011 studied the electron transport process into dimensional graphene system and Peres (2010) investigated graphene transport mechanism and conductivity behavior. Using the tight binding and density functional calculations, research by Pereira at al., (2009) and Roberto et al.,(2009) also show our strain and lattes information affect graphene electronic characteristics. Also using density functional theory techniques, Agbolade et al., 2024 examine the optoelectronic and magnetic properties of graphene systems doped with brown and beryllium. A notable changes in BAND structural behavior were found and are prominent to nano electronic applications. Likewise Zhang et al., (2022) studied competition, graphene systems for electronic structure, utilizing first principles method. Reich et al. (2002) investigated the electronic structure of graphene using an enhanced tight-binding model. Their study demonstrated that incorporating interactions up to the third-nearest neighbors significantly improved the accuracy of the calculated electronic band structure compared with the conventional nearest-neighbor approximation, providing a more reliable description of graphene's electronic properties. The aim of this research is to use the nearest neighbor tight binding approximation to computationally, analyze the electrical band structures of graphene and to build its reciprocal lattice representation, access the graphene energy, dispersion relation numerically, visualize the villain and conduction energy bands and examine the electronic consequences of graphene zero band gap semimetallic behavior.

METHODOLOGY AND THEORETICAL FRAMEWORK

The electronic band structure of graphene was studied using a competition Condensed matter physics method based on the nearest neighborhood tight binding approximation. This method integrates numerical simulations which was carried out utilizing python models with a theoretical explanation of Graphene's honeycomb lattice. The process was intended to visualize the conduction and various energy band, replicate the electron dispersion relation of graphene and explore its appearance of the distinctive Dirac cone structure linked to relativistic like charge carriers. Two interpenetrating triangular sub lattice open, referred to as A and B mix up the hexagonal honeycomb lattice structure of graphene (Castro Neto et al., 2009). The remaining p_z orbital contributes to the delocalized π-electron system that gives graphene its unique electrical characteristics, while each carbon atom generates three strong sp^2 hybridized σ bonds with nearby atoms. The graphene crystal structure's primitive lattice vectors are provided by:

$$\overrightarrow{a}_1 = a\left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right), \quad \overrightarrow{a}_2 = a\left(\frac{3}{2}, -\frac{\sqrt{3}}{2}\right)$$

where a is the carbon-carbon bond length within the lattice. The periodic arrangement of atoms in the graphene crystal generates a corresponding reciprocal lattice representation that governs electron motion in momentum space.

The reciprocal lattice vectors associated with graphene are expressed as

$$\overrightarrow{b}_1 = \frac{2\pi}{3a}(1, \sqrt{3}), \quad \overrightarrow{b}_2 = \frac{2\pi}{3a}(1, -\sqrt{3})$$

The electrical structure was numerically assessed by discretizing reciprocal space coordinates over finite intervals according to:

$$k_x \in [-\pi, \pi], \quad k_y \in [-\pi, \pi]$$

After that, Python were used to numerically construct the reciprocal space coordinates. The graphene energy dispersion relation was then assessed through momentum space using a two-dimensional reciprocal lattice meshgrid.

To calculate the electrical structure, the nearest-neighbor tight-binding approximation was used. This approximation was chosen cause it offers an effective and physically accurate description of π-electron interactions in graphene (Wallace, 1947; Saito et al., 1998). Electron hopping was limited to carbon atoms that were closest to one another inside the tight-binding framework. The tight-binding Hamiltonian for graphene is provided by

$$H = -t\sum_{\langle i,j \rangle}(a_i^\dagger b_j + b_j^\dagger a_i)$$

where t represents the nearest-neighbor hopping parameter, while $a_i^\dagger$ and $b_j^\dagger$ denote electron creation operators associated with the two graphene sublattices. The notation $\langle i, j \rangle$ represents nearest-neighbor interactions between adjacent carbon atoms. The application of Bloch's theorem to the periodic graphene lattice yielded the electronic energy dispersion relation expressed as

$$E(k) = \pm t \sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_y a}{2}\right)\cos\left(\frac{k_x a}{2}\right) + 4\cos^2\left(\frac{k_x a}{2}\right)}$$

The valence band is represented by the negative branch of the dispersion relation, whereas the conduction band is represented by the positive branch. The Dirac cones that are typical of graphene arise from the intersection of both branches at particular symmetry positions within the Brillouin zone.

The dispersion relation becomes roughly linear close to the Dirac points and can be expressed as

$$E(k) \approx \hbar v_F |k|$$

where $\hbar$ is the reduced Planck constant, v_F denotes the Fermi velocity, and k represents the wave vector measured relative to the Dirac point. This linear energy-momentum relationship explains the relativistic-like behavior of charge carriers in graphene.

All numerical simulations were performed using Python. The simulations employed the NumPy library for numerical calculations and array manipulations, Matplotlib was used for scientific visualization and graphical representation of the computed energy bands. To numerically evaluate the graphene dispersion relation, reciprocal space coordinates were generated using discretized arrays according to

$$k_x = linspace(-\pi, \pi, N), \quad k_y = linspace(-\pi, \pi, N)$$

where N represents the number of discretization points used in the simulation. The reciprocal space meshgrid was subsequently constructed using

$$(K_x, K_y) = meshgrid(k_x, k_y)$$

The generated meshgrid provided the numerical coordinate system required for evaluating the graphene energy surfaces throughout reciprocal space.

The conduction and valence energy bands were numerically computed by substituting the reciprocal space coordinates into the graphene dispersion relation according to

$$E_{\pm} = \pm t \sqrt{1 + 4\cos\left(\frac{\sqrt{3}K_y a}{2}\right)\cos\left(\frac{K_x a}{2}\right) + 4\cos^2\left(\frac{K_x a}{2}\right)}$$

When simulating, normalize value of the lattice, constant and hopping parameters were used for the computation. Both two dimensional and three dimensional charting approaches were used to visualize the electrical structure. The topology of the conduction and valence bands was depicted using three dimensional surface plots, and the symmetry and periodicity of the graphing passional relation in reciprocal space were well examined using contour plots. In investigating the linear discussion behavior more localized visualization close to the Dirac points were created. These features were seen as indicators of the semi metallic property and exceptionally high carrier mobility of graphene. In order to validate the numerical implementation, the generated bank structure were finally qualitatively compared with previously established investigations which was reported in the research literature.

RESULTS AND DISCUSSION

The electronic band structure derived from the tight-binding simulation is presented in Figs. 1–3. The computational results confirm the validity of the nearest-neighbor tight-binding approximation, which is fundamental for describing low-energy π-electron interactions in the graphene honeycomb lattice. The simulated band structure accurately reproduces the distinctive electronic characteristics of graphene reported in theoretical and experimental studies.

Figure 1 presents the calculated three-dimensional band structure of graphene over the first Brillouin zone. The results reveal two distinct energy surfaces corresponding to the valence and conduction bands. Both surfaces exhibit strong symmetry about the zero-energy plane (E = 0), demonstrating the electron-hole symmetry inherent in the graphene lattice. The valence band extends into the negative energy region (E < 0), whereas the conduction band occupies the positive energy region (E > 0). As the momentum approaches the high-symmetry points in reciprocal space, the two bands continuously converge until they meet. The calculated energy range extends from approximately − 3.0eV to + 3.0 eV, while the colour distribution provides a quantitative representation of the energy variation throughout the Brillouin zone. One of the most significant physical observations from Fig. 1 is the absence of a finite energy band gap between the valence and conduction bands. The continuous intersection of the two bands at the K and K' points, where the energy is exactly zero (E = 0), confirms the semimetallic nature of graphene. Unlike conventional semiconductors, in which electrons must overcome a finite band gap, typically between 0.5 and 3.0 eV, before electrical conduction can occur, graphene exhibits direct band contact that enables charge carriers to move with negligible excitation energy. The calculated band gap of 0.0 eV therefore confirms the gapless electronic structure of graphene, which is primarily responsible for its exceptionally high electrical conductivity and carrier mobility exceeding 200,000 cm²/V·s. Furthermore, the electronic dispersion is clearly non-parabolic throughout the Brillouin zone. In contrast to conventional crystalline materials, where the energy varies quadratically with momentum $(E \propto k^2)$, the calculated energy surfaces exhibit significant deviations from parabolic behaviour, particularly near the band-contact regions where the dispersion becomes linear $(E \propto |k|)$. Consequently, the conventional effective mass approximation, which typically yields effective masses of about 0.05–0.10me in ordinary semiconductors, is no longer appropriate because the effective mass approaches zero near the Dirac points.

A magnified view of the electronic energy spectrum in the vicinity of the band-contact region is presented in Fig. 2. The numerical results clearly reveal the characteristic conical energy structure known as the Dirac cone. Around the Fermi level (E = 0), the energy varies approximately linearly with momentum according to the relation

$$[E = \pm \hbar\, v_F |k|,]$$

where $(v_F = 10^6)$ m/s represents the Fermi velocity. Owing to the finite numerical resolution of the simulation, the apex of the cone appears slightly rounded, which results from the discretization of the reciprocal-space grid into 200 × 200 points for computational stability. Nevertheless, the overall linearity of the dispersion remains well preserved. These results demonstrate that the low-energy quasiparticles in graphene behave as relativistic-like massless Dirac fermions rather than conventional electrons with parabolic dispersion. The linear dispersion is maintained throughout the low-energy region $(|E| < 1.0eV)$, confirming that Dirac-like dynamics govern charge transport in graphene. The slope of the simulated Dirac cone yields a Fermi velocity of approximately (1.0×10^6)m/s, which agrees closely with theoretical predictions for pristine graphene. This relativistic-like behaviour explains several remarkable electronic properties that have been experimentally observed, including ballistic electron transport with mean free paths exceeding 1μm at room temperature, suppression of back-scattering arising from the centrality of Dirac fermions, and exceptionally high electron mobility greater than 200,000 cm²/V·s. The emergence of the Dirac cone directly results from the geometric symmetry of the graphene honeycomb lattice and the nearest-neighbour hopping interaction incorporated into the tight-binding Hamiltonian using a hopping parameter of (t = 2.8) eV. These findings demonstrate that graphene's unusual electronic properties are intrinsic consequences of its lattice geometry rather than externally induced effects.

The contour representation of the graphene energy spectrum in reciprocal space is shown in Fig. 3. The contour map displays a highly symmetric energy distribution centred within the Brillouin zone. Smooth and continuous contour patterns are observed throughout the reciprocal-space domain, reflecting the gradual variation of electronic energy with crystal momentum and confirming the numerical stability of the calculated band structure. Near the central region, the contour lines appear nearly circular because of the finite reciprocal-space window and numerical discretization adopted in the simulation, with contour intervals of 0.3 eV.

The gradual transition from the high-energy region (E ≈ + 3.0 eV) to the low-energy region (E ≈ − 3.0 eV) illustrates the continuous nature of graphene's dispersion relation. At the centre of the contour map (k = 0), the energy is approximately + 3.0 eV, whereas movement towards the K points $((k = \pm 2\pi/3a))$ results in a continuous reduction of energy until it reaches 0.0 eV. This behaviour clearly illustrates the linear dispersion that characterizes the electronic structure near the Dirac points. The contour lines remain uniformly spaced around these points, providing additional confirmation of the linear relationship

$$[E = \pm \hbar\, v_F |k\,|]$$

within the low-energy regime. The calculated bandwidth of approximately 6.0 eV, extending from − 3.0 eV to + 3.0 eV, is in excellent agreement with both first-principles calculations and experimental measurements reported in the literature.

The results provide a consistent physical description of graphene as a two-dimensional semimetal possessing a zero band gap and relativistic-like electronic dispersion. The numerical simulations demonstrate that the nearest-neighbour tight-binding approximation accurately captures the essential electronic properties of graphene while maintaining computational efficiency. The quantitative analysis of the simulated band structure reveals several important electronic parameters. The hopping integral, (t = 2.8) eV, determines the overall energy bandwidth, while the Fermi velocity,

$$[v_F = \frac{3ta}{2\hbar} \approx \ 1.0 \times \ 10^6 \, m/s,]$$

is directly obtained from the slope of the Dirac cone. The linear dispersion around the Dirac points remains valid for energies satisfying |E| < 1.0 eV, corresponding to momentum values $|k - kD| < 0.3\text{Å}^{-1}$. The calculations further demonstrate exact electron-hole symmetry throughout the Brillouin zone, with the valence and conduction bands forming perfect mirror images about E = 0. In addition, the density of electronic states near the Dirac point varies linearly with energy, $(\rho(E) \propto |E|)$, unlike the constant density of states characteristic of conventional two-dimensional electron gases. These quantitative results confirm that the nearest-neighbour tight-binding model provides an accurate, physically consistent, and computationally efficient description of graphene's electronic structure, making it well suited for further investigations of charge transport phenomena and graphene-based electronic device applications.

CONCLUSION

Graphene's electronic band structure was investigated computationally using the nearest-neighbor tight-binding approximation, focusing on its low-energy electronic behavior in reciprocal space. The symmetrical valence and conduction bands, the zero band gap of 0.0 eV, and the appearance of almost linear dispersion close to the Dirac regions were successfully replicated in the simulated results, with the calculated Dirac cone confirming a Fermi velocity of vF ≈ 1.0 × 10⁶ m/s and a total bandwidth of approximately 6.0 eV. These characteristics verify that graphene is semimetallic and that its low-energy π-electron dynamics can be accurately described by the nearest-neighbor tight-binding approximation. The Dirac-like energy structures shown in the calculated band spectrum confirm that the electrical characteristics of graphene are essentially controlled by lattice symmetry and electron hopping interactions within the honeycomb crystal structure. Graphene's importance as a model system that links relativistic quantum mechanics and condensed matter physics through the emergence of massless quasiparticles is further supported by this relativistic-like dispersion behavior. This research establishes graphene as a physically significant platform for understanding the connection between crystal symmetry, electronic transport properties, and band topology in condensed matter physics, as well as a foundation for investigating quantum electronic behavior in two-dimensional systems. The

computational approach established here provides a robust framework for future investigations of graphene-based devices and the extension to more complex carbon allotropes.

Declarations

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AUTHOR CONTRIBUTIONS

Iyanuoluwa O. Ajayi: Conceptualization, methodology, software, formal analysis, investigation, data curation, visualization, writing, original draft preparation.

Samuel O. Adeosun: Simulation, Data analysis.

Tolulope A. Ojuola: Supervision, Proof reading.

DECLARATIONS

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Ethics Approval: Not Applicable

Competing Interest: The author declares there is no competing interest as regards this research

Code Availability: The Python and MATLAB codes used for the numerical simulations and visualization are available from the corresponding author upon request.

Data Availability: The datasets generated and analyzed during this research are available from the corresponding author upon reasonable request.

Consent to Publish declaration: Not applicable.

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CORRESPONDING AUTHOR

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Figures

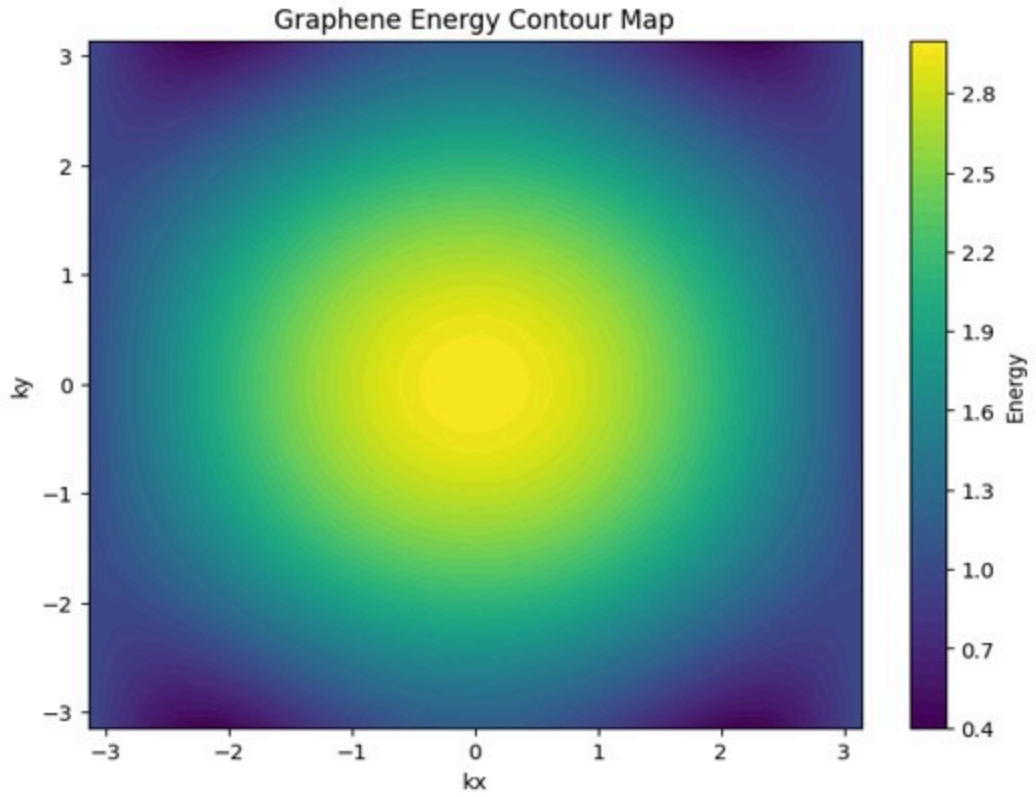


Figure 1

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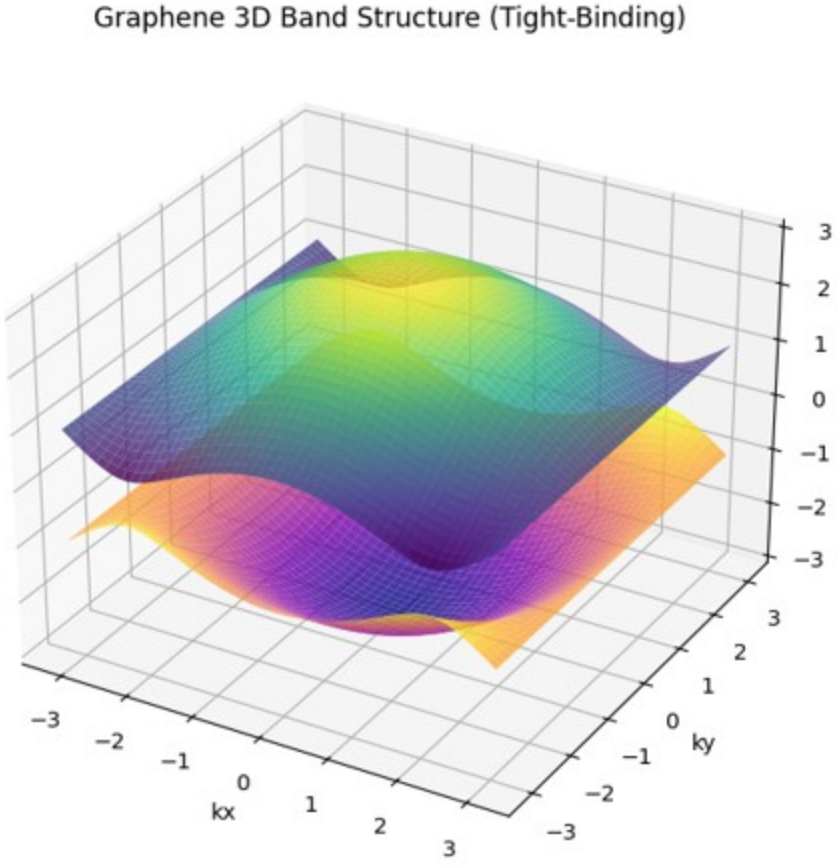


Figure 2

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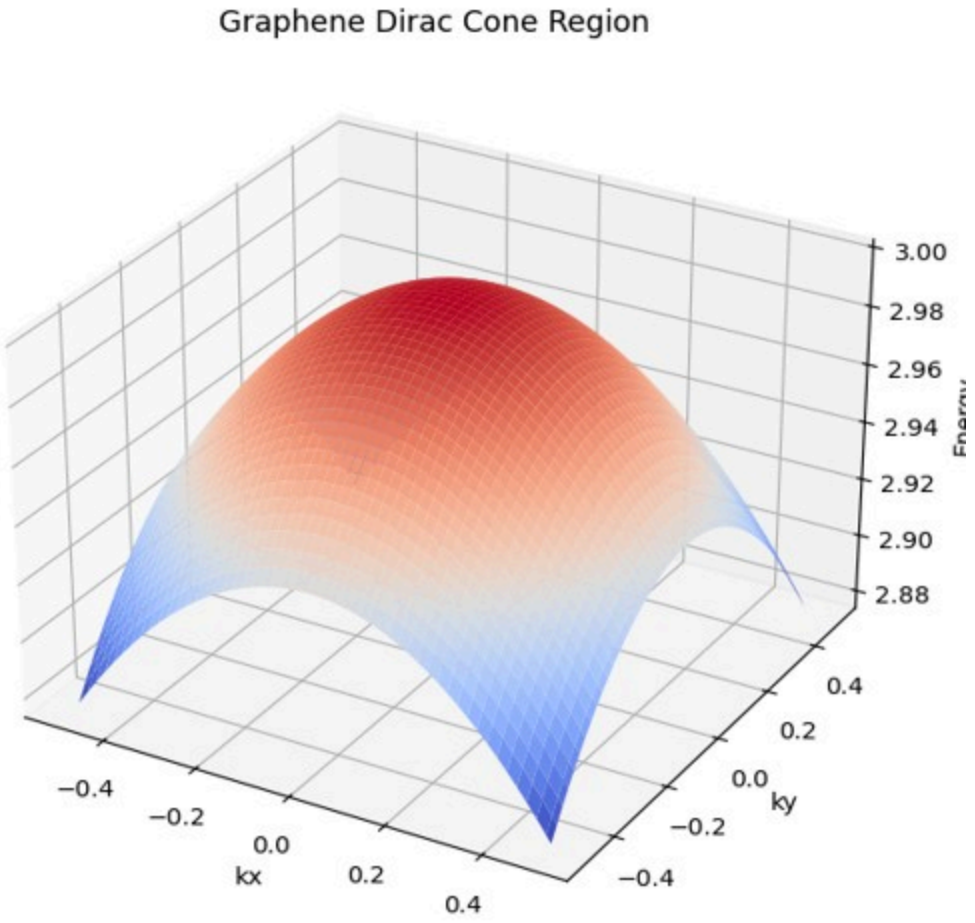


Figure 3

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