Heatmaps of NNN-Driven Asymmetry in Graphene

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We investigate electron–hole asymmetry in monolayer graphene using a **minimal π-band tight-binding model** that adds Next-Nearest-Neighbor (NNN) hopping to the standard nearest-neighbor (NN) Hamiltonian. While NN hopping alone yields **particle–hole symmetry and a Dirac crossing at charge neutrality**, a finite NNN term preserves the gapless crossing but shifts the neutrality point and skews band curvatures across the Brillouin zone. We quantify these effects with two complementary outputs: (i) band overlays along Γ–K–M–Γ that show the Dirac crossing moving rigidly with the NNN term and the loss of spectral mirror symmetry; and (ii) a Brillouin-zone **"asymmetry map,"**.

Symmetry in Graphene

• Graphene Structure: Single layer of carbon atoms in a two-dimensional honeycomb lattice. • Bonding in Graphene: Strong covalent bonds between carbon atoms, with planar structure and sp^2 hybridization. • Electronic Properties: π bonding is crucial for understanding electron energy levels in graphene.

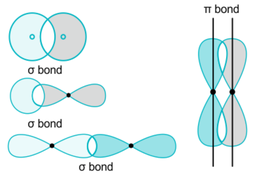


Figure 1. Out-of-plane π bonding

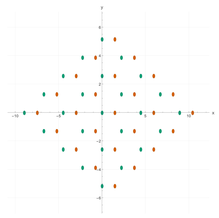


Figure 2. A(Green) and B(Orange) Sublattices.

The (Minimal) Band Structure of Graphene

Solving the Schrödinger Equation with NNN and π orbitals, we obtain a solvable $2x2$ matrix. With a possible sublattice offset Δ (set $\Delta = 0$ for graphene), the two bands are

$$E_{\pm}(\mathbf{k}) = \frac{\Delta}{2} + \frac{(t_{2A} + t_{2B})}{2} g(\mathbf{k}) \pm \sqrt{\left[\frac{\Delta}{2} + \frac{(t_{2A} - t_{2B})}{2} g(\mathbf{k})\right]^2 + t^2 |\gamma(\mathbf{k})|^2} \quad (1)$$

$$\boxed{E_{\pm}(\mathbf{k}) = t_2\, g(\mathbf{k}) \pm t\, |\gamma(\mathbf{k})|} \quad (2)$$

• Parameters: t and t_2 represents the NN and NNN parameters respectively. • Adjusting the last parameter allows observation of changes in the band structure.

Calculations were performed in Wolfram Mathematica, and the code is available at `https://kimreyesg.github.io/research.html`.

The Band structure of Graphene

(Incomplete but correct)

Using the minimal model NNN Tight Binding it is able to reproduce the two most important bands of Graphene, the Valence Band Maximum (VBM) and Conduction Band Minimum (CBM).

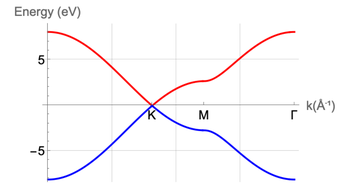


Figure 3. Tight binding band structure of graphene considering just nearest-neighbor (NN) ($t_2 = 0$).

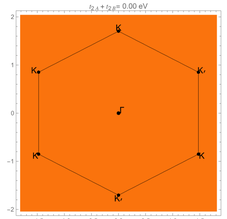


Figure 4. NNN Symmetry field $A(\mathbf{k})$. $t_2 = 0$ Perfect symmetric conduction and valence band

Global energy shift (not doping) If $t_2 > 0$ the whole spectrum moves downward by $3t_2$; if $t_2 < 0$ it moves upward by $3|t_2|$. This *looks* like changing the Fermi level, but it is *not* doping: in an undoped, isolated sheet the Fermi level E_F stays at the band touching, so $E_F = E_D$ and both move together (E_D Dirac Energy).

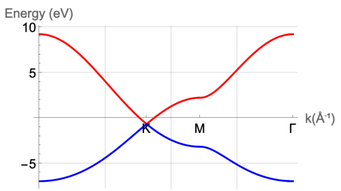


Figure 5. Graphene NNN tight-binding bands with $t_2 = +0.20$ eV.

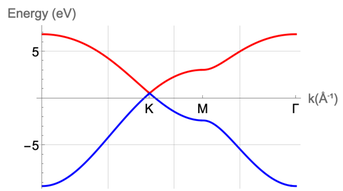
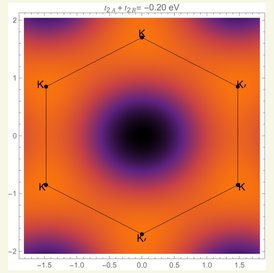


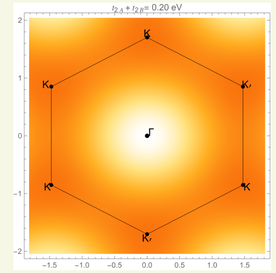
Figure 6. Graphene NNN tight-binding bands with $t_2 = -0.20$ eV.

The asymmetry field $A(\mathbf{k})$ Definition (centered at the Dirac energy): $A(\mathbf{k}) = E_+ + E_-$.

$$\boxed{A(\mathbf{k}) = (t_{2A} + t_{2B})\,\big[g(\mathbf{k}) + 3\big].} \quad (3)$$



(a) Graphene heat map with $t_2 = -0.10$ eV.



(b) Graphene heat map with $t_2 = +0.10$ eV.

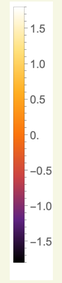


Figure 7. Next–nearest–neighbor asymmetry field $A(\mathbf{k})$ for opposite signs of t_2 (fixed color scale shared by both panels).

Final Results

- Regions where $A(\mathbf{k}) \approx 0$ indicate nearly perfect electron–hole symmetry; expect equal slopes and nearly equal curvatures of the two branches.
- Regions with large $|A(\mathbf{k})|$ flag where electron and hole effective masses will differ most strongly at matched energy distances from the Dirac energy; this influences mobility, quantum capacitance, and the position of van Hove features.

References

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