Calibrating Tight Binding for Biaxially Strained Graphene

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We study the effect of **uniform biaxial strain** on monolayer graphene using a minimal **tight-binding model** with nearest and next-nearest neighbor hopping, treating the carbon–carbon distance a as a strain parameter while keeping hopping amplitudes t and t_2 fixed. This strain-independent parametrization fails to match experimental trends. We introduce a distance-dependent hopping $t(a)$ of **exponential form at equilibrium**. This modification significantly enhances the model's accuracy in describing the strain dependence of low-energy observables in graphene over a realistic biaxial strain range.

How can we strain graphene?

Graphene is a semimetal with a honeycomb lattice of carbon atoms. At equilibrium, the carbon–carbon bond length is ($a_0 = 1.42$ Å) and the band structure is gapless. We varied from $a = 1.36$ Å (compressive strain) to $a = 1.56$ Å (tensile strain).

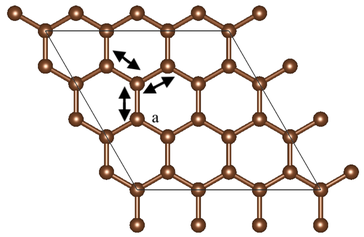

Figure 1. Graphene: a honeycomb lattice of carbon atoms.

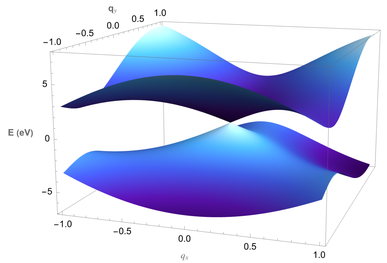

Figure 2. Energy E versus crystal momentum $\mathbf{k}$ near the K point of graphene's Brillouin zone ($a = 1.42$ Å).

Two Tight Binding Models

The band structure of graphene is distinctive because it exhibits a **Dirac cone** at the K point. Under uniform biaxial strain, we study how this Dirac cone changes within the tight–binding approximation using two models:

- **Model A (geometry-only strain):** the bond length a changes with strain, while the hopping parameters t and t_2 are kept fixed.
- **Model B (distance-dependent hopping):** the bond length a changes with strain, and the hopping parameters decay with distance,

$$t(a) = t_0 \exp\left[-\beta\left(\frac{a}{a_0} - 1\right)\right], \qquad t_2(a) = t_{2,0} \exp\left[-\beta\left(\frac{a}{a_0} - 1\right)\right].$$

We employ a minimal tight-binding model that includes both nearest- and next-nearest-neighbor interactions.

Why strain matters

around the Dirac cone...

Under uniform biaxial strain, the carbon–carbon bond length a changes. In a next-nearest neighbor (NNN) tight binding (TB) model with distance-dependent hopping, stretching ($a \uparrow$) reduces orbital overlap and typically lowers the slope of the cone (Fermi velocity), while compression ($a \downarrow$) increases it. Graphene is gapless at K, so the conduction and valence bands touch and form a cone-like dispersion.

Comparison of graphene Dirac cones using the two parameterizations: constant t versus $t(a)$.

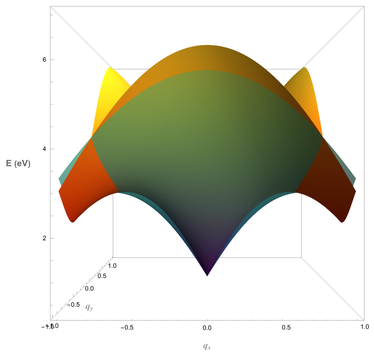

Figure 3. 3D Dirac cones for extreme biaxial strain ($a = 1.36$ Å compression and $a = 1.56$ Å tension) using the NNN tight-binding model with constant t

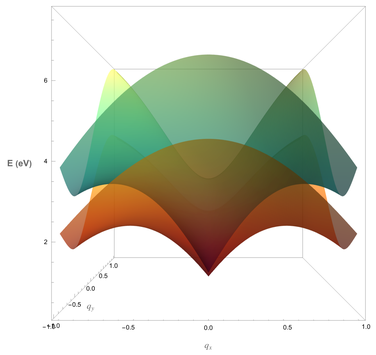

Figure 4. 3D Dirac cones for the same strains using distance-dependent hopping $t(a)$ (and $t_2(a)$)

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

Fermi velocity from the Dirac cone (tight binding) Near a Dirac point K, the dispersion is approximately linear:

$$E_+(\mathbf{K} + \mathbf{q}) \approx \hbar v_F |\mathbf{q}|.$$

Therefore, the Fermi velocity is the slope of the conduction cone at K:

$$v_F = \frac{1}{\hbar} \frac{\partial E_+}{\partial |\mathbf{q}|}\bigg|_{\mathbf{q}=0}$$

In the nearest-neighbor tight-binding model this gives the standard result:

$$v_F = \frac{3at}{2\hbar}$$

where a is the C–C bond length and t is the nearest-neighbor hopping.

Table 1. Fermi velocity for different biaxial strains in graphene.

a (Å)	$\varepsilon = (a - a_0)/a_0$ (%)	v_F (constant t, $10^5\,\mathrm{m\,s^{-1}}$)	v_F ($t(a)$, $10^5\,\mathrm{m\,s^{-1}}$)
1.36	−4.2	8.37	9.65
1.42	0.0	8.74	8.74
1.56	+9.9	9.60	6.89

Final Results

- **Unstrained check:** We obtain $v_F(a_0) \approx 8.7 \times 10^5\,\mathrm{m\,s^{-1}}$, within $\sim 10\%$–20% of the commonly quoted $v_F^{\mathrm{exp}} \sim (1.0\text{–}1.1) \times 10^6\,\mathrm{m\,s^{-1}}$.
- **Why the offset is expected:** A minimal nearest and next-nearest neighbor tight binding model (with $t_0 = 2.7\,\mathrm{eV}$) omits many-body and environmental effects (substrates, screening).
- **Model B is better:** Distance-dependent hopping $t(a)$ accounts for reduced orbital overlap under tension and corrects the qualitative strain trend (the constant-t model can predict an unrealistic increase of v_F with tensile strain).

References

[1] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim. The electronic properties of graphene. *Reviews of Modern Physics*, 81(1):109–162, 2009. doi: 10.1103/RevModPhys.81.109.

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