Electronic Edge States in Graphene Sheets

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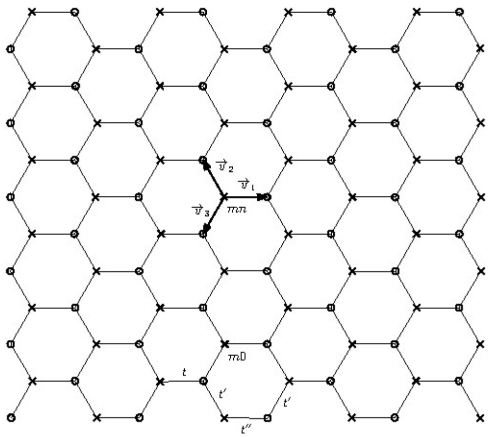


2D Honeycomb of C: identical, not "symmetrically-identical"

Graphene: ideal, "clean" Dirac electronic spectrum; strong (hard), both on substrate or independent

Instability: finite size (purely quantum solids?)

Motivation:

1) finite-size ribbons, there exist edges

2) usually semiconducting - only edge states active

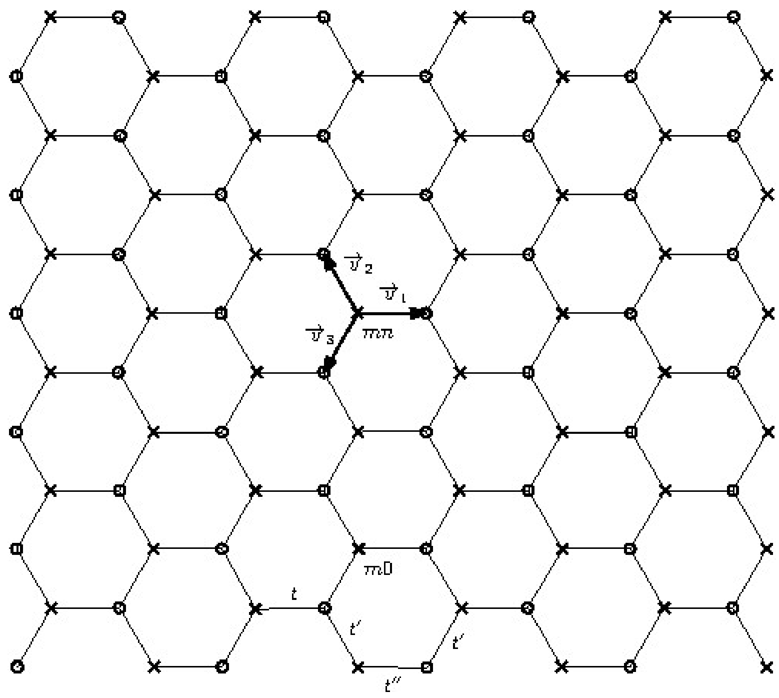
3) can be controlled (?)

4) photo-excited in photovoltaics (?)

Presentation:

Simple, analytical calculations for edge states

Infinite sheet



Atom (m, n) and $\mathbf{v}_{1,2,3}$; periodicity: twice the vectors $\mathbf{v}_{1,2,3}$

Tight-binding amplitudes a_{mn} and $b^{\mathbf{v}}_{mn}$:

$$\varepsilon a_{mn} = t(b^{\mathbf{v}_1}_{mn} + b^{\mathbf{v}_2}_{mn} + b^{\mathbf{v}_3}_{mn}) \ ,$$

$$\varepsilon b^{\mathbf{v}_1}_{mn} = t^*(a_{mn} + a^{\mathbf{v}_1-\mathbf{v}_2}_{mn} + a^{\mathbf{v}_1-\mathbf{v}_3}_{mn}) \ ,$$

$$\varepsilon b^{\mathbf{v}_2}_{mn} = t^*(a_{mn} + a^{\mathbf{v}_2-\mathbf{v}_1}_{mn} + a^{\mathbf{v}_2-\mathbf{v}_3}_{mn}) \ ,$$

$$\varepsilon b^{\mathbf{v}_3}_{mn} = t^*(a_{mn} + a^{\mathbf{v}_3-\mathbf{v}_2}_{mn} + a^{\mathbf{v}_3-\mathbf{v}_1}_{mn})$$

Periodic solutions $a^{\mathbf{v}}_{mn} \sim A(\mathbf{K})e^{i\mathbf{K}[(m,n)+\mathbf{v}]}$, $b^{\mathbf{v}}_{mn} \sim B(\mathbf{K})e^{i\mathbf{K}[(m,n)+\mathbf{v}]}$, $\mathbf{K} = (k, q)$

Energies ($\lambda = \varepsilon/t$):

$$|\lambda|^2 = 3 + 2\cos\mathbf{K}(\mathbf{v}_1 - \mathbf{v}_2) + 2\cos\mathbf{K}(\mathbf{v}_1 - \mathbf{v}_3) + 2\cos\mathbf{K}(\mathbf{v}_2 - \mathbf{v}_3)$$

$$|\lambda|^2 = \varepsilon^2/\,|t|^2 = 1 + 4\cos\frac{3k}{2}\cos\frac{\sqrt{3}q}{2} + 4\cos^2\frac{\sqrt{3}q}{2}$$

Amplitudes:

$$\lambda A = B(e^{i\mathbf{K}\mathbf{v}_1} + e^{i\mathbf{K}\mathbf{v}_2} + e^{i\mathbf{K}\mathbf{v}_3})\ ,\ \lambda^* B = A(e^{-i\mathbf{K}\mathbf{v}_1} + e^{-i\mathbf{K}\mathbf{v}_2} + e^{-i\mathbf{K}\mathbf{v}_3})$$

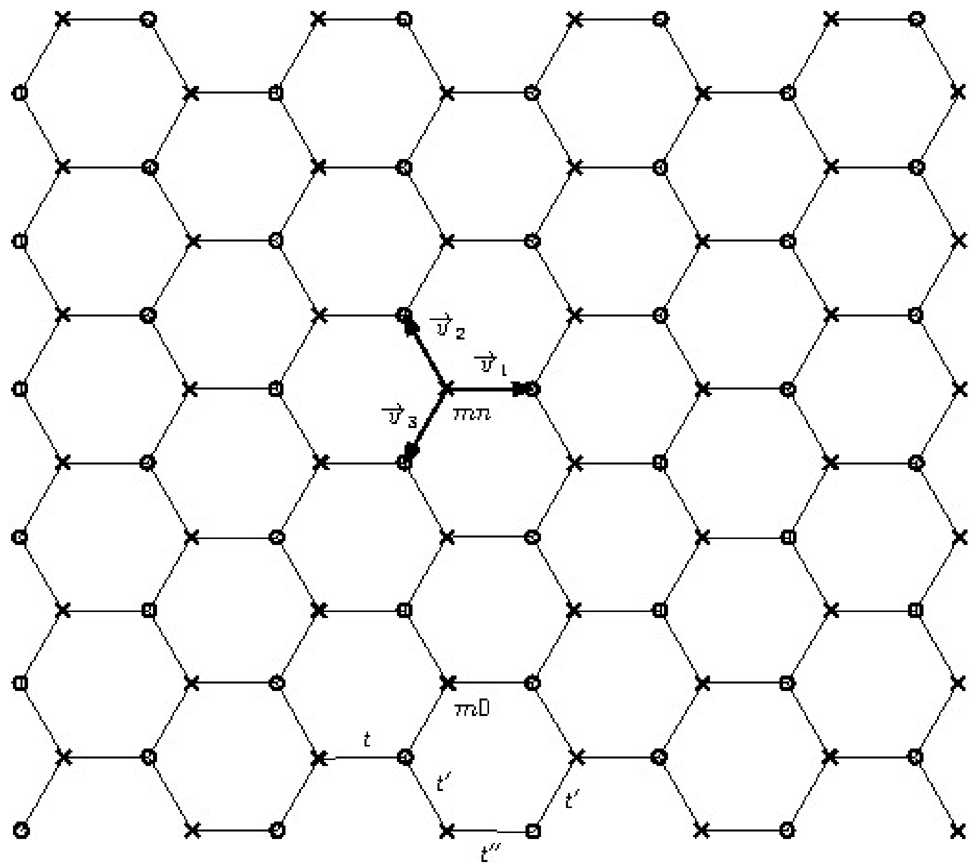
Energy $\varepsilon = \pm t\sqrt{S}$,

$$S = 1 + 4\cos\frac{3k}{2}\cos\frac{\sqrt{3}q}{2} + 4\cos^2\frac{\sqrt{3}q}{2}$$

S is positive over the BZ, hexagon $3k/2 = \pm\pi$, $\sqrt{3}q/2 = \pm\pi/3$, $k = 0$, $\sqrt{3}q/2 = \pm 2\pi/3$; $S = 9$ at the centre of BZ $S = 0$ at the hexagon corners

Vertices BZ: $\varepsilon = \pm(3t/2)K$, $\mathbf{K} = (k, q)$ **gapless Dirac** (Wallace 1947)

Armchair edge



Transfer matrix **modified** at the edge (Tamm 1932, Shockley 1939)

$$\varepsilon b_{m0}^{\mathbf{v}_3} = t(a_{m0} + a_{m0}^{\mathbf{v}_3-\mathbf{v}_1}) + t' a_{m0}'^{\mathbf{v}_3-\mathbf{v}_2} \ ,$$

$$\varepsilon a_{m0}^{\mathbf{v}_1-\mathbf{v}_2} = t(b_{m0}^{\mathbf{v}_1} + b_{m0}^{2\mathbf{v}_1-\mathbf{v}_2}) + t' b_{m0}'^{\mathbf{v}_1-\mathbf{v}_2+\mathbf{v}_3} \ ,$$

$$\varepsilon a_{m0}'^{\mathbf{v}_3-\mathbf{v}_2} = t' b_{m0}^{\mathbf{v}_3} + t'' b_{m0}'^{\mathbf{v}_3-\mathbf{v}_2+\mathbf{v}_1} \ ,$$

$$\varepsilon b_{m0}'^{\mathbf{v}_1-\mathbf{v}_2+\mathbf{v}_3} = t' a_{m0}^{\mathbf{v}_1-\mathbf{v}_2} + t'' a_{m0}'^{\mathbf{v}_3-\mathbf{v}_2} \ ;$$

Boundary condition ($\lambda = \varepsilon/t$, $t' = t(1+\sigma)$, $t'' = t(1+\rho)$):

$$\rho e^{i\frac{3k}{2}} + \sigma(2+\sigma)e^{-\frac{\sqrt{3}q}{2}} - e^{\frac{\sqrt{3}q}{2}} = 0$$

Edge states: $\mathbf{K} = (k,q) \to (k,iq)$: **No solution**

Semi-infinite sheet with perfect edges: $\sigma = 0$, $\rho = 0$, $A^{'} = A$, $B^{'} = B$
"Reflected" solution

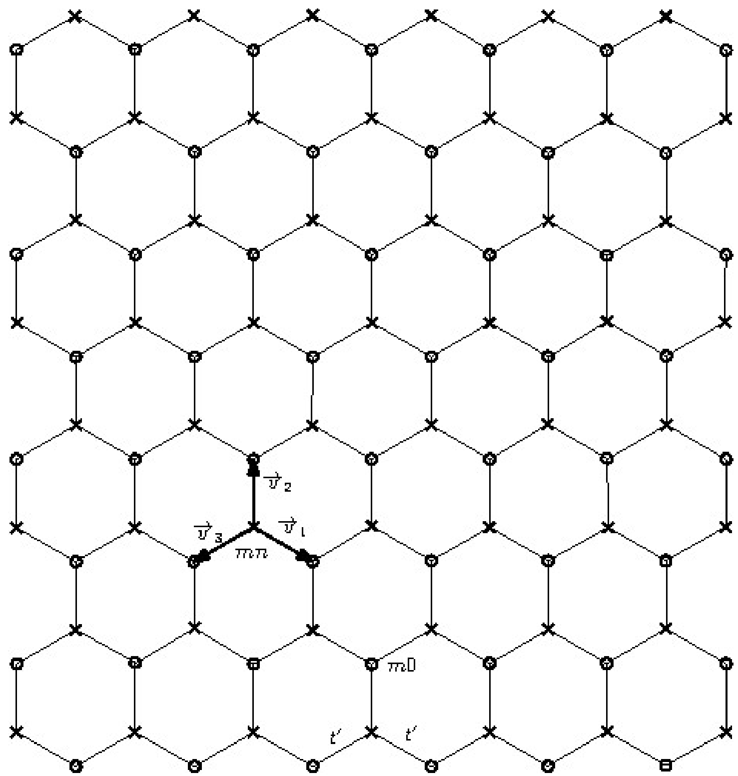
$$Ae^{ik(m+v_x)} \sin q(n - \sqrt{3}/2 + v_y) \ , \ Be^{ik(m+v_x)} \sin q(n + \sqrt{3}/2 + v_y)$$

Ancient Work and Method:

Corciovei 1960-1970 (founder of Th Phys in Romania) (ferromagnetism, elastic chain)

Brillouin 1930s

Zig-zag edge



Equations:

$$\varepsilon a_{m0}^{-\mathbf{v}_2} = t b_{m0} + t' b'^{-\mathbf{v}_2+\mathbf{v}_1}_{m0} + t' b'^{-\mathbf{v}_2+\mathbf{v}_3}_{m0} \ ,$$

$$\varepsilon b'^{-\mathbf{v}_2+\mathbf{v}_1}_{m0} = t' a_{m0}^{-\mathbf{v}_2} + t' a_{m0}^{-\mathbf{v}_2+\mathbf{v}_1-\mathbf{v}_3} \ ,$$

$$\varepsilon b'^{-\mathbf{v}_2+\mathbf{v}_3}_{m0} = t' a_{m0}^{-\mathbf{v}_2} + t' a_{m0}^{-\mathbf{v}_2-\mathbf{v}_1+\mathbf{v}_3}$$

Boundary condition:

$$2\sigma(2+\sigma)\cos\frac{\sqrt{3}k}{2} = e^{-i\frac{3q}{2}} \rightarrow e^{3q/2}$$

Solutions $q \rightarrow iq$ (damped) for $-1-\sqrt{2}/2 < \sigma < -1+\sqrt{2}/2$, or $\sigma < -1-\sqrt{6}/2$, $\sigma > -1+\sqrt{6}/2$

We conclude: semi-infinite graphene sheet with zig-zag edge has edge states, propagating plane waves along the direction parallel with the edge (wavevector k) and damped waves along the direction perpendicular to the edge ($\sim e^{-q(n+v_y)}$), for values of (k, q) given by equation above

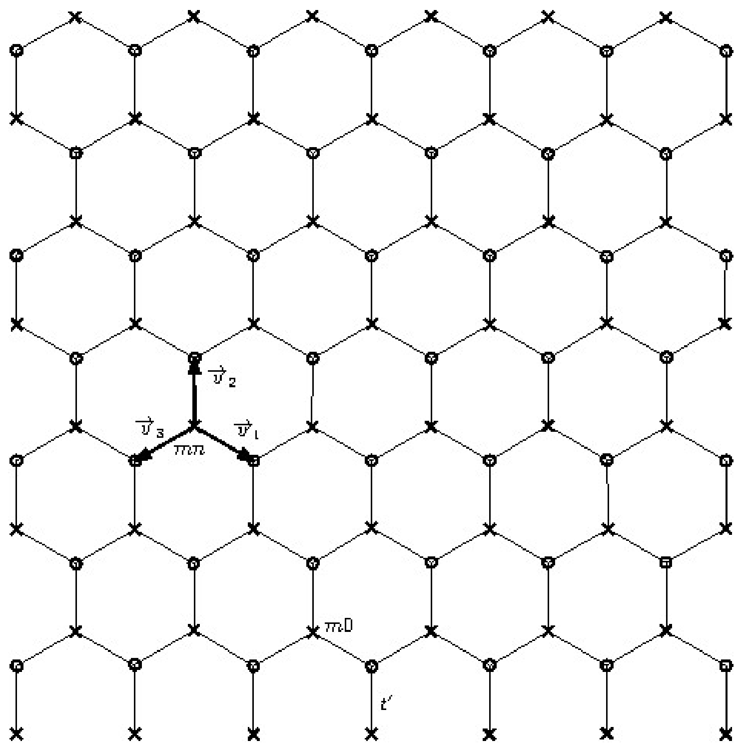
Energy (in the gap):

$$\lambda^2 = 1 + 4\cosh\frac{3q}{2}\cos\frac{\sqrt{3}k}{2} + 4\cos^2\frac{\sqrt{3}k}{2} =$$

$$= \left[1 + \frac{1}{\sigma(2+\sigma)}\right]\left[1 + \frac{1}{\sigma(2+\sigma)}e^{3q}\right]$$

$(0 < q < \frac{2}{3}\ln|2\sigma(2+\sigma)|)$; for each q two k's

Horseshoe edge



Unrealistic: dangling bonds terminate with hydrogen, blocked

Equations

$$\varepsilon b^{\mathbf{v}_1}_{m0} = t(a_{m0} + a^{\mathbf{v}_1-\mathbf{v}_3}_{m0}) + t' a'^{\mathbf{v}_1-\mathbf{v}_2}_{m0} \ ,$$

$$\varepsilon a'^{\mathbf{v}_1-\mathbf{v}_2}_{m0} = t' b^{\mathbf{v}_1}_{m0}$$

Solutions:

$$\frac{1}{2}\sigma(2+\sigma)e^{-\frac{3q}{2}} = \cos\frac{\sqrt{3}k}{2}$$

Two k's for each q in $q = \frac{2}{3}\ln\left|\frac{1}{2}\sigma(+\sigma)\right|$, provided $\sigma < -1 - \sqrt{3}$ or $\sigma > -1 + \sqrt{3}$

Energy

$$\lambda^2 = (1+\sigma)^2\left[1 + \sigma(2+\sigma)e^{-3q}\right]$$

Ribbon: two zig-zag edges (N rows)

Reflected solutions: $(A_1, B_1)e^{-qn} + (A_2, B_2)e^{-q(N-n)}$

Same solution

etc,etc