Graphene ribbon 1-D band structure

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Zigzag ribbon

The tight-banding hamiltonian for graphene is taken as[1]

$$H = -t \sum_{\text{n.n.},\sigma} \left(a_i^\dagger b_j + \text{h.c.} \right) - t' \sum_{\text{n.n.n.},\sigma} \left(a_i^\dagger a_j + b_i^\dagger b_j + \text{h.c.} \right)$$

The zigzag ribbon is taken to be infinite in the x direction and finite in the y direction. The sums are now rewritten as a sum over sets of lattice sites that are translationally invariant in the x direction and finite in the y direction. The set of sites is taken to be one of the "zigzag" paths starting at the top of the nanoribbon and ending at the bottom. Suppose it goes from top-right to bottom-left. Abandon the $a^\dagger, b^\dagger$ notation and label the sites sequentially: $a_{j,1,\sigma}^\dagger,\ a_{j,2,\sigma}^\dagger,\ \ldots$.

First, the nearest-neighbor sum. Consider set j. The odd-numbered sites couple to set $j+1$ and the even-numbered sites couple to set $j-1$. Specifically, $a_{j,i,\sigma}^\dagger$ couples to $a_{j+1,i+1,\sigma}$ if i is odd, and to $a_{j-1,i-1,\sigma}$ if i is even. Additionally, each of the sites along within j will couple to its other neighbors in j.

Suppose there are N full honeycomb cells in the y direction. The nearest-neighbor sum may then be rewritten as

$$-t \sum_{\text{n.n.},\sigma} \left(a_i^\dagger b_j + \text{h.c.} \right) = -t \sum_{j,\sigma} \left[H_j^I + \frac{1}{2} \sum_{i=1}^{N+1} \left(a_{j,2i-1,\sigma}^\dagger a_{j+1,2i,\sigma} + a_{j,2i,\sigma}^\dagger a_{j-1,2i-1,\sigma} \right) + \text{h.c.} \right]$$

where H_j^I is the contribution from tunnelling between lattice sites on the same j:

$$H_j^I = a_{j,1,\sigma}^\dagger a_{j,2,\sigma} + a_{j,2,\sigma}^\dagger a_{j,3,\sigma} + \ldots a_{j,2N+1,\sigma}^\dagger a_{j,2N+2,\sigma}.$$

In Fourier space, the nearest-neighbor terms takes the form

$$\begin{aligned} H_{\text{n.n.}} &= -t \sum_{k,\sigma} \left[H_k^I + \frac{1}{2} \sum_{i=1}^{N+1} \left(a_{k,2i-1,\sigma}^\dagger a_{k,2i,\sigma} e^{ik\sqrt{3}a/2} + a_{k,2i,\sigma}^\dagger a_{k,2i-1,\sigma} e^{-ik\sqrt{3}a/2} \right) + \text{h.c.} \right] \\ &= -t \sum_{k,\sigma} \left[(H_k^I + \text{h.c.}) + \sum_{i=1}^{N+1} \left(a_{k,2i-1,\sigma}^\dagger a_{k,2i,\sigma} e^{ik\sqrt{3}a/2} + a_{k,2i,\sigma}^\dagger a_{k,2i-1,\sigma} e^{-ik\sqrt{3}a/2} \right) \right]. \end{aligned}$$

Here,

$$H_k^I = a_{k,1,\sigma}^\dagger a_{k,2,\sigma} + a_{k,2,\sigma}^\dagger a_{k,3,\sigma} + \ldots + a_{k,2N+1,\sigma}^\dagger a_{k,2N+2,\sigma}$$

[1] "Electronic properties of graphene"

Hence, the $(2N+2)\times(2N+2)$ matrix representation of $H_{\text{n.n.}}(k)$ takes the form

$$H_{\text{n.n.}} = -t \begin{pmatrix} 0 & 1+e^{ik\sqrt{3}a/2} & 0 & & 0 & 0 \\ 1+e^{-ik\sqrt{3}a/2} & 0 & 1+e^{ik\sqrt{3}a/2} & \cdots & 0 & 0 \\ 0 & 1+e^{-ik\sqrt{3}a/2} & 0 & & 0 & 0 \\ & \vdots & & \ddots & & \\ 0 & 0 & 0 & & 0 & 1+e^{ik\sqrt{3}a/2} \\ 0 & 0 & 0 & & 1+e^{-ik\sqrt{3}a/2} & 0 \end{pmatrix}.$$

The eigenvalues of this Toeplitz tridiagonal matrix may be computed analytically. The determinant of the first 3×3 block is given by

$$-\lambda^2 - 2|a|^2\lambda,$$

where $a = 1 + e^{ik\sqrt{3}a/2}$.