An analytical approach to the spectrum of π electrons in bilayer graphene nanoribbons and nanotubes

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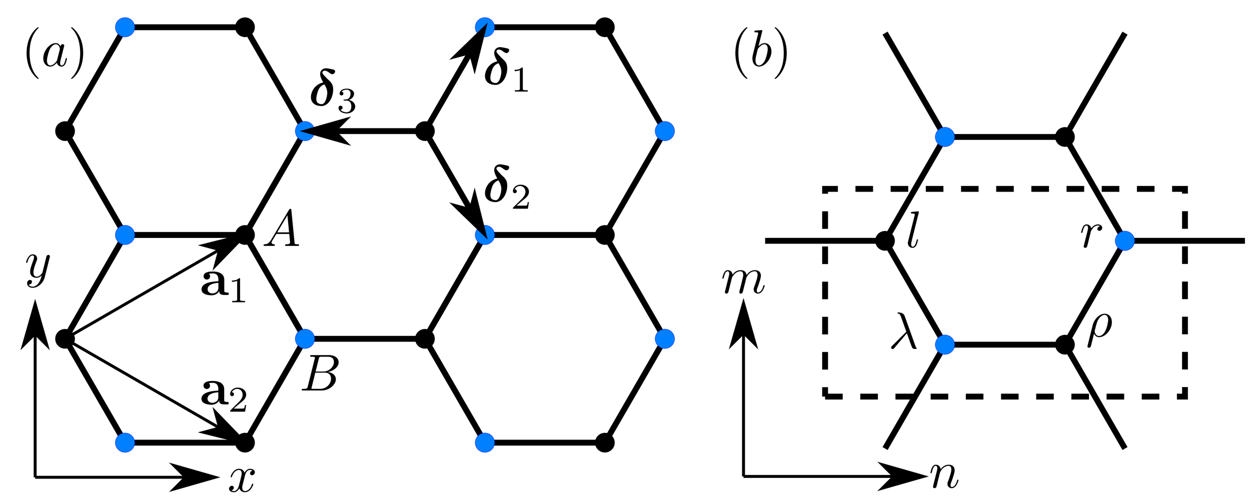
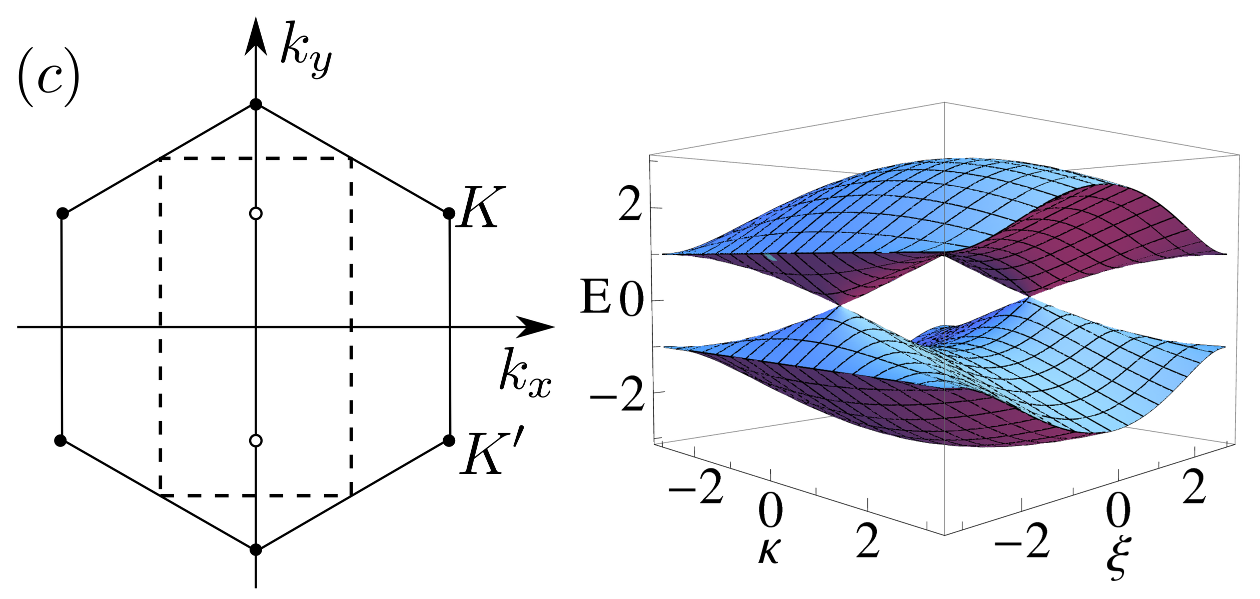
Abstract

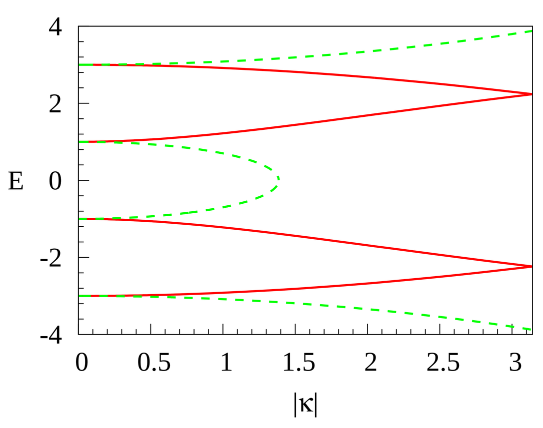
We present an analytical description of π electrons of a finite size bilayer graphene within a framework of the tight-binding model. The considered bilayered structures are characterized by a rectangular geometry and have a finite size in one or both directions with armchair- and zigzag-shaped edges. An exact analytical description of the spectrum of π electrons in the zigzag and armchair bilayer graphene nanoribbons and nanotubes is provided. The exact solution of the Schrödinger problem, the spectrum and wave functions, has been obtained and used to analyze the density of states and the conductance quantization.

[1] J. Ruseckas, G. Juzeliūnas, and I. V. Zozoulenko, *Spectrum of electrons in bilayer graphene nanoribbons and nanotubes: An analytical approach*, Phys. Rev. B **83**, 035403 (2011).

Single layer graphene







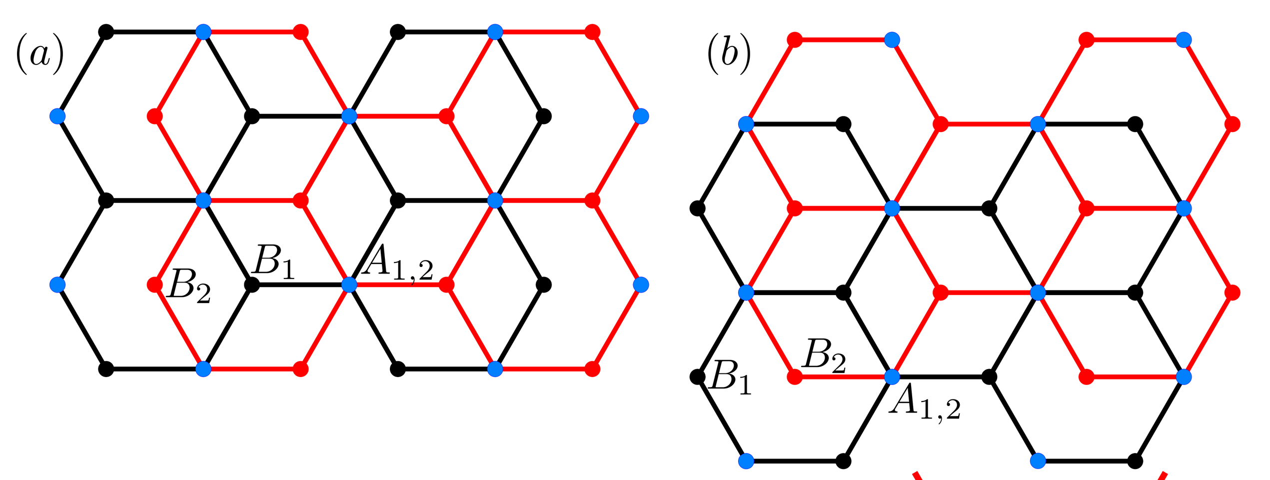
The tight-binding Hamiltonian for electrons in graphene:

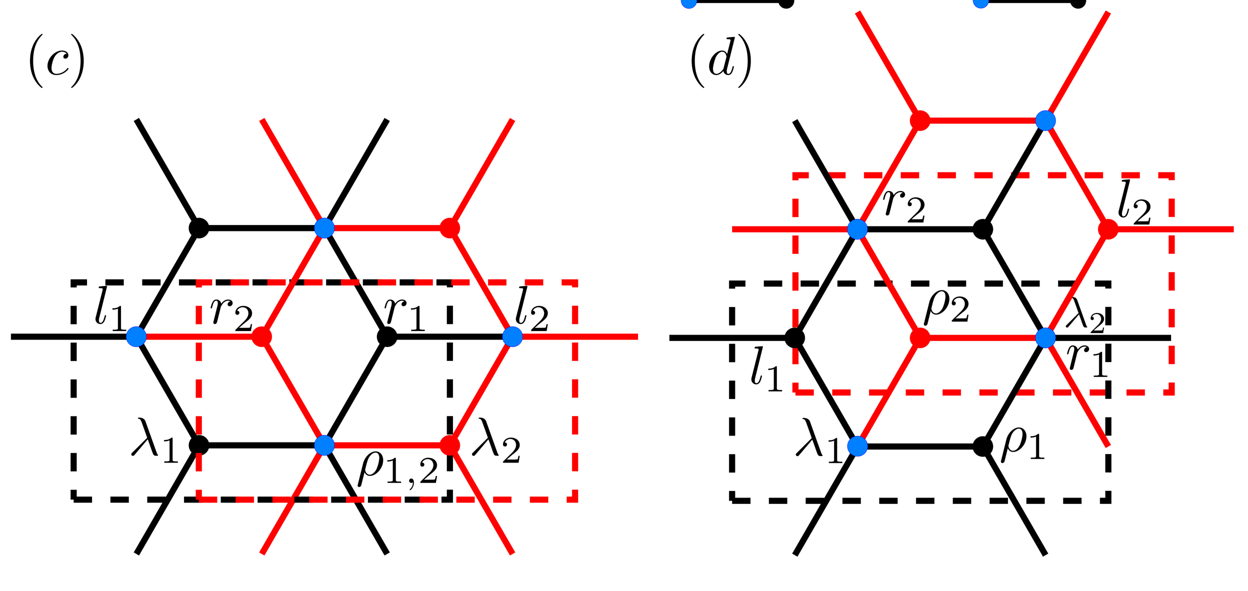
$$H_{\mathrm{gr}} = -t\sum_{\langle i,j\rangle}(a_i^\dagger b_j + b_j^\dagger a_i)$$

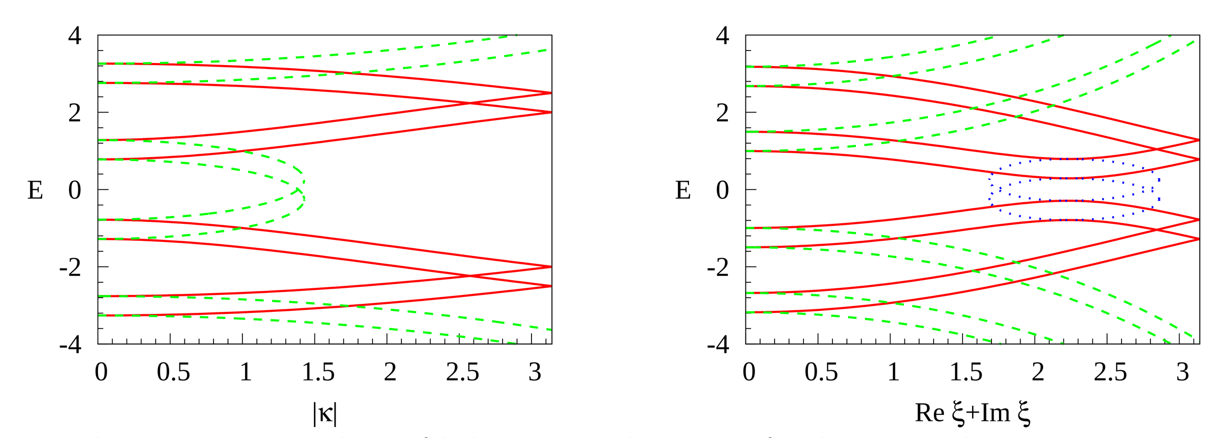
Rectangular unit cell: the area of the Brillouin zone is two times smaller than the area of the Brillouin zone of the hexagonal unit cell.
In rectangular structures: condition for wave vectors

$$\frac{\sin(\kappa N)}{\sin(\kappa(N+1/2))} = -s_3 2\cos(\xi_j/2)$$

Bilayer graphene







Lower part: dispersion branches of bilayer graphene. Left: $\xi = 0$; right: $\kappa = 1.0$

The minimal model of the tight-binding Hamiltonian for electrons in bilayer graphene:

$$H_{\mathrm{bi}} = -t\sum_{\langle i,j\rangle,p}(a^\dagger_{i,p}b_{j,p} + b^\dagger_{j,p}a_{i,p}) - t_\perp\sum_j(a^\dagger_{j,1}a_{j,2} + a^\dagger_{j,2}a_{j,1}) + V\sum_j(a^\dagger_{j,2}a_{j,2} + b^\dagger_{j,2}b_{j,2} - a^\dagger_{j,1}a_{j,1} - b^\dagger_{j,1}b_{j,1})$$

Dimensionless Cartesian components of the wave vector: $\kappa = 3ak_x$, $\xi = \sqrt{3}ak_y$
Eigenvectors in the form of plane waves: $\psi_{m,n,\alpha} = c_\alpha e^{i\xi m + i\kappa n}$
Example: For AB-α stacking and $V = 0$ coefficients of the eigenvectors are

$$c_{r_1} = 1\,,\quad c_{\rho_1} = -e^{-i\frac{\xi}{2}}\frac{E(\kappa,\xi)}{\phi(-\kappa,\xi)}\,,\quad c_{l_1} = -s_3 e^{-i\frac{\xi}{2}}\frac{E(\kappa,\xi)}{\phi(-\kappa,\xi)}\,,\quad c_{\lambda_1} = s_3 e^{-i\frac{1}{2}(\kappa+\xi)}\,,$$
$$c_{r_2} = -s_1 s_2\frac{\phi(\kappa,\xi)}{\phi(-\kappa,\xi)}\,,\quad c_{\rho_2} = s_1 s_2 e^{-i\frac{\xi}{2}}\frac{E(\kappa,\xi)}{\phi(-\kappa,\xi)}\,,\quad c_{l_2} = s_1 s_2 s_3 e^{i\frac{\xi}{2}}\frac{E(\kappa,\xi)}{\phi(-\kappa,\xi)}\,,$$
$$c_{\lambda_2} = -s_1 s_2 s_3 e^{i\frac{1}{2}(\kappa-\xi)}\frac{\phi(\kappa,\xi)}{\phi(-\kappa,\xi)}\,;\qquad \phi(\kappa,\xi) = s_3 e^{-i\frac{\kappa}{2}} + 2\cos(\xi/2)$$

Electron spectrum in infinite sheet of bilayer graphene:

$$E(\kappa,\xi) = s_1\sqrt{\frac{\gamma^2}{2} + V^2 + |\phi(\kappa,\xi)|^2 + s_2\sqrt{\frac{\gamma^4}{4} + |\phi(\kappa,\xi)|^2(4V^2+\gamma^2)}}$$

For $V = 0$:

$$E(\kappa,\xi) = s_1\left(s_2\frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{4} + |\phi(\kappa,\xi)|^2}\right)\;;\quad |\phi(\kappa,\xi)|^2 = 1 + 4\cos^2\left(\frac{\xi}{2}\right) + s_3 4\cos\left(\frac{\xi}{2}\right)\cos\left(\frac{\kappa}{2}\right)$$

Here $s_1, s_2, s_3 = \pm 1$ and $\gamma \equiv t_\perp/t \approx 0.14$.
There are two eigenstates with wave vectors $\kappa^{(1)}$ and $\kappa^{(2)}$ corresponding the same energy: $E(\kappa^{(1)},\xi) = E(\kappa^{(2)},\xi)$. Condition for signs: $s_1^{(2)}s_2^{(2)} = -s_1^{(1)}s_2^{(1)}$. When $V = 0$:

$$s_3^{(2)}\cos(\kappa^{(2)}/2) = s_3^{(1)}\cos(\kappa^{(1)}/2) + s_1^{(1)}s_2^{(1)}\frac{\gamma}{2\cos(\xi/2)}E(\kappa^{(1)},\xi)$$

Rectangular structures of bilayer graphene: N rectangular unit cells in the x (armchair) direction and $\mathcal{N}+1/2$ rectangular unit cells in the y (zigzag) direction, so that there are $\mathcal{N}$ hexagons along the y axis. We search for the eigenvectors of the Hamiltonian as a superposition of plane waves obeying boundary conditions.
Example: For AB-α stacking and $V = 0$ the possible values of ξ_j are

$$\xi_j = \frac{\pi j}{\mathcal{N}+1}\,,\qquad j = 1,\ldots,\mathcal{N}+1$$

and the possible values of $\kappa^{(1)}_{j,\nu_j}$ are solutions of one of the equations

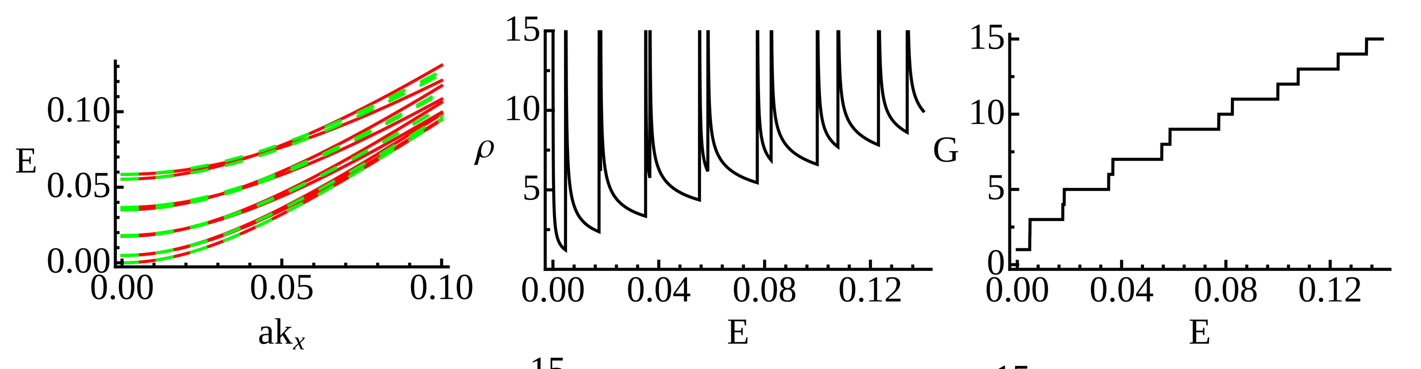
$$1 + \cos\left(\frac{\xi}{2}\right)\left(s_3^{(1)}\frac{\cos\left(\frac{1}{2}\kappa^{(1)}(N+1)\right)}{\cos\left(\frac{1}{2}\kappa^{(1)}N\right)} + s_3^{(2)}\frac{\sin\left(\frac{1}{2}\kappa^{(2)}(N+1)\right)}{\sin\left(\frac{1}{2}\kappa^{(2)}N\right)}\right) = 0$$
$$1 + \cos\left(\frac{\xi}{2}\right)\left(s_3^{(1)}\frac{\sin\left(\frac{1}{2}\kappa^{(1)}(N+1)\right)}{\sin\left(\frac{1}{2}\kappa^{(1)}N\right)} + s_3^{(2)}\frac{\cos\left(\frac{1}{2}\kappa^{(2)}(N+1)\right)}{\cos\left(\frac{1}{2}\kappa^{(2)}N\right)}\right) = 0$$

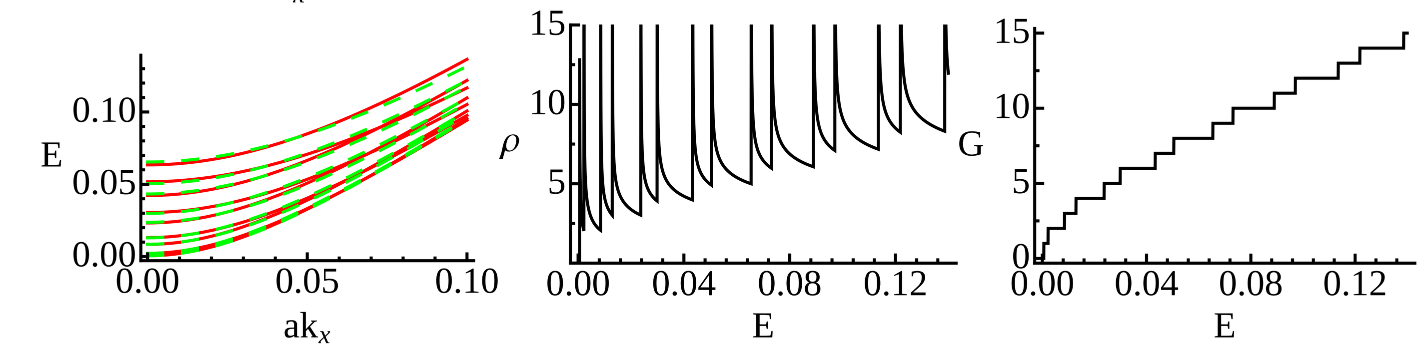
Band structure near the Fermi energy

The band structure of bilayer graphene tubes and ribbons when $V = 0$ near the Fermi energy

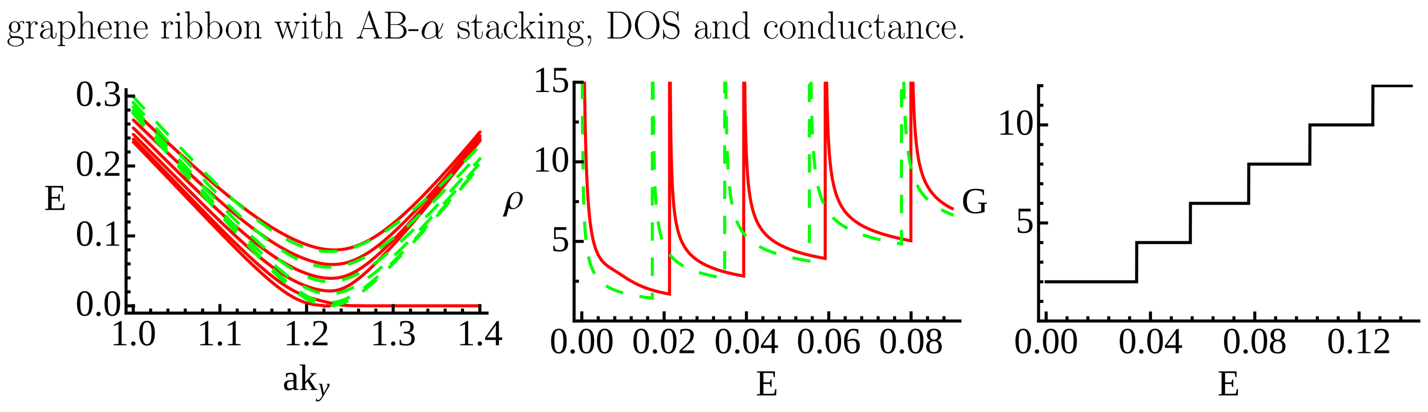
$$E_\nu(k_\parallel) \approx s_1\left(-\frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{4} + \frac{9}{4}a^2[(k_\parallel - \bar{k}^\sigma_\parallel)^2 + k^{\sigma 2}_{\perp\nu}]}\right)$$

$k_\parallel$ and $k_{\perp\nu}$ are the longitudinal and the transverse components of the wave vector.





Upper part: band structure of metallic armchair bilayer graphene ribbon with AB-α stacking, DOS and conductance. Lower part: band structure of semiconducting armchair bilayer graphene ribbon with AB-α stacking, DOS and conductance.



Band structure of zigzag bilayer graphene ribbon with AB-α stacking, DOS and conductance.