Electronic Properties of Graphene Nanoribbons in Magnetic Field

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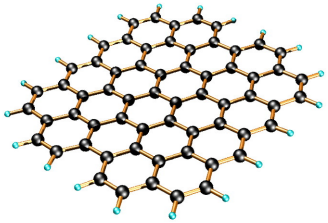
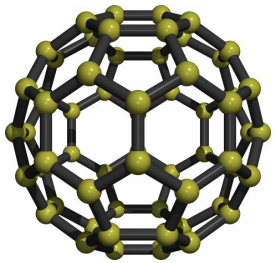
Electronic Properties of Graphene Nanoribbons in Magnetic Field

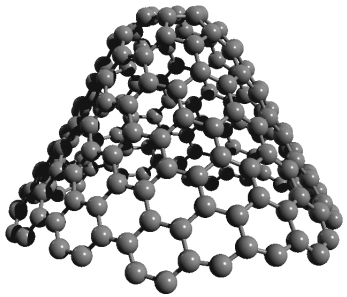
- Carbon Nanostructures:
  - graphene



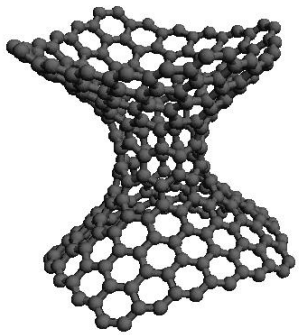
  - fullerene



  - nanocone

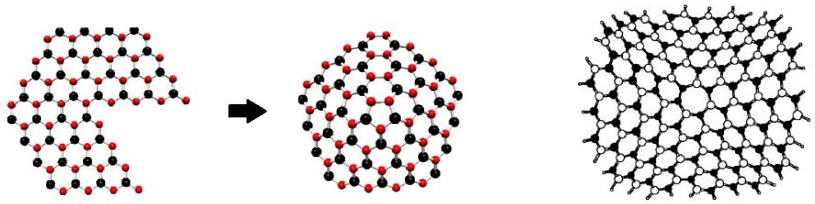


  - wormhole

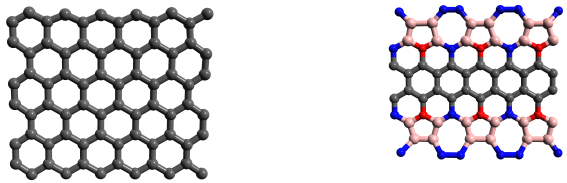


Electronic Properties of Graphene Nanoribbons in Magnetic Field

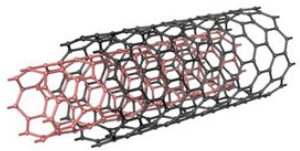
- vicinity of defects



- nanoribbon



- double-walled nanotubes

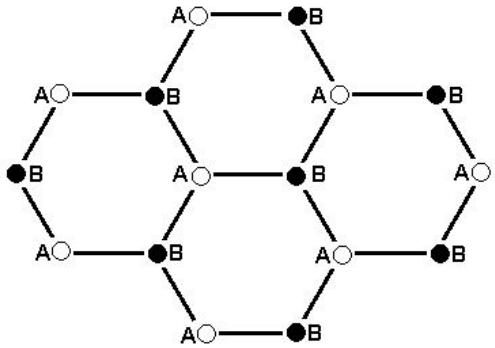


- single-walled nanotubes, nanotoroids, etc.

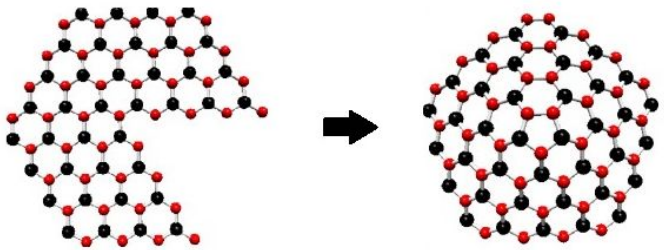
Electronic Properties of Graphene Nanoribbons in Magnetic Field

- Basic structure: Hexagonal plain lattice

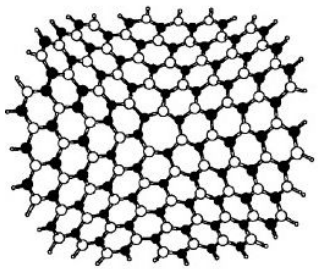
  it is composed of 2 inequivalent sublattices, *A* and *B*



- Topological defects: *n*-sided polygons



$n \leq 5$ (positive curvature)



$n \geq 7$ (negative curvature)

Electronic Properties of Graphene Nanoribbons in Magnetic Field

- Electronic properties
  - Important characteristics: Local density of states

    number of states per the unit interval of energy and per the unit area of surface at each energy level that is available to be occupied by electrons
  - Calculation of *LDoS* for low energies:
    - periodical structures: from the low energy electronic spectrum using Schrödinger equation describing the electron motion [1,2]
    - aperiodical structures: from the continuum limit of the gauge field theory using Dirac-like equation describing the motion of massless fermion [3]
    - graphene wormhole: using Dirac-like equation describing the motion of massive fermion [4]

Electronic Properties of Graphene Nanoribbons in Magnetic Field

- Periodical structures: plain graphene (continuous spectrum), fullerene, nanotubes, nanoribbons (discrete spectrum)
  - the electron which is bounded on the molecular surface satisfies the Schrödinger equation [1]:

$$H\psi = E\psi, \qquad \psi = C_{A_1}\psi_{A_1} + ... + C_{A_{n_{max}}}\psi_{A_{n_{max}}}$$

    where $A_1, ..., A_{n_{max}}$ represent the sublattices created by the particular atom sites in the unit cell
  - solution: Bloch function $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u_{\vec{k}}(\vec{r})$, where $u_{\vec{k}}(\vec{r})$ has the lattice periodicity [5]
  - tight-binding approximation:

$$\psi_{A_i} = \sum_{A_i} \exp[i\vec{k}\cdot\vec{r}_{A_i}]X(\vec{r}-\vec{r}_{A_i}),$$

    where $X(\vec{r})$ is the atomic orbital function, one can verify that ψ_{A_i} satisfies the Bloch theorem for the sublattice A_i
  - assumption: $\int X(\vec{r}-\vec{r}_{A_i})X(\vec{r}-\vec{r}_{A_j})\mathrm{d}\vec{r} = 0$ for $i \neq j$

Electronic Properties of Graphene Nanoribbons in Magnetic Field

- case of graphene
  - we denote

$$H_{ab} = \int \psi_a^* H \psi_b \mathrm{d}\vec{r}, \qquad S = \int \psi_A^* \psi_A \mathrm{d}\vec{r} = \int \psi_B^* \psi_B \mathrm{d}\vec{r}, \qquad a, b \equiv A, B,$$

  then

$$\begin{pmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{pmatrix} \begin{pmatrix} C_A \\ C_B \end{pmatrix} = ES \begin{pmatrix} C_A \\ C_B \end{pmatrix}$$

  - the lattice symmetry gives $H_{AA} = H_{BB}$, $H_{AB} = H_{BA}$, then, putting $H'_{ab} = H_{ab}/S$, we get the secular equation

$$\begin{vmatrix} H'_{AA} - E & H'_{AB} \\ H'_{AB} & H'_{AA} - E \end{vmatrix} = 0,$$

    from which follows $E = H'_{AA} \pm |H'_{AB}|$
  - we consider H'_{AA} to be the Fermi level, then, after substitution the corresponding expansion into H'_{AB}, we get

$$E(\vec{k}) = \pm\gamma_0 \sqrt{1 + 4\cos^2\frac{k_y a}{2} + 4\cos\frac{k_y a}{2}\cos\frac{k_x a\sqrt{3}}{2}},$$

Electronic Properties of Graphene Nanoribbons in Magnetic Field

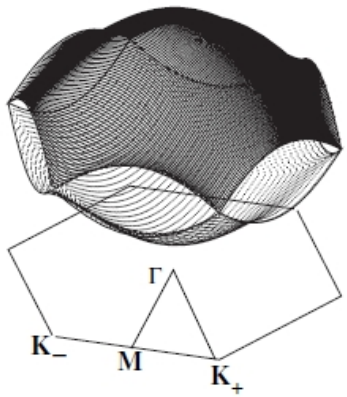
where

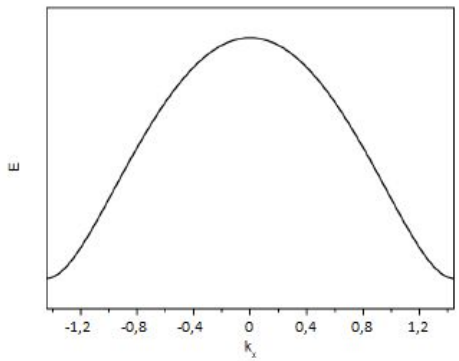
$$\gamma_0 = -\int X^*(\vec{r} - \vec{\rho}) H X(\vec{r}) \mathrm{d}\vec{r},$$

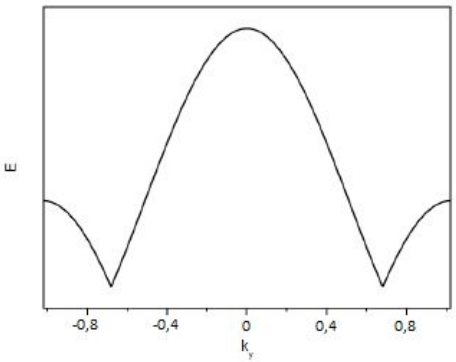
$\vec{\rho}$ joining the given site A with the nearest site B

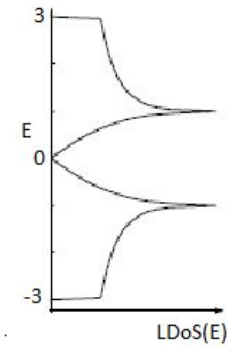
- the *LDoS* we get as

$$LDoS(E,k) = \frac{\delta(E - E(k))}{D(E)}, \qquad D(E) = \lim_{\eta \to 0} 2\mathrm{Im} \int_{-\pi}^{\pi} \mathrm{d}k \frac{k}{E - E(k) - i\eta}$$



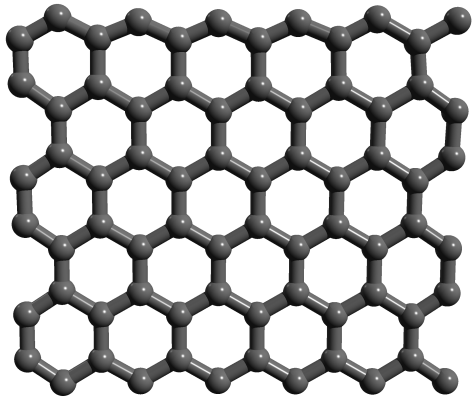


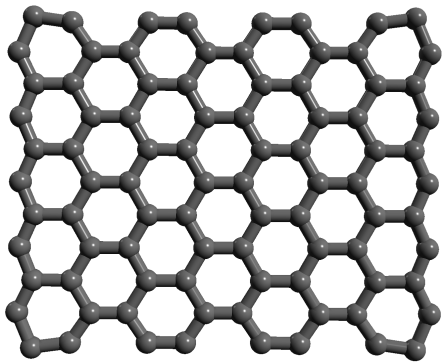




Electronic Properties of Graphene Nanoribbons in Magnetic Field

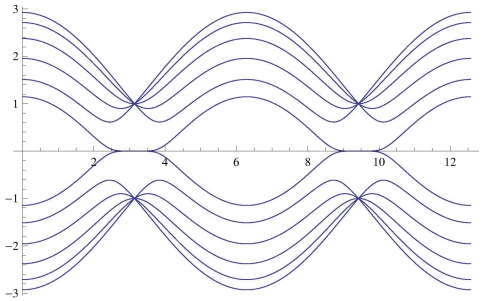
- different kinds of nanoribbons
  - these nanostructures have high variability - their properties can be influenced by the changes of width and edge structure
  - they are 2 basic types with different electronic properties: zigzag (metal) and armchair (semimetal)

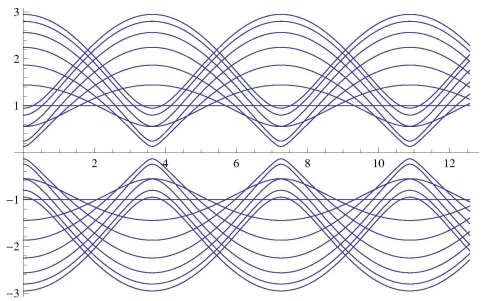




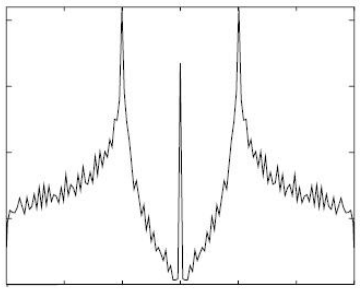
Electronic Properties of Graphene Nanoribbons in Magnetic Field

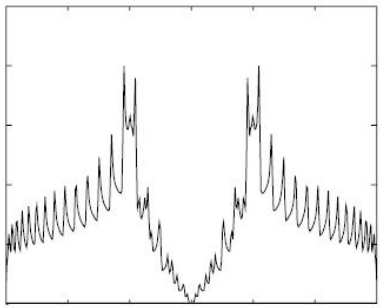
- around zero, it creates either a localized state (case of metals) or a gap (case of semimetals); the width of the gap can be influenced by different admixtures





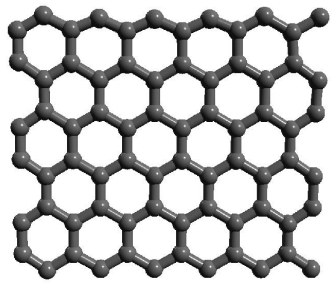
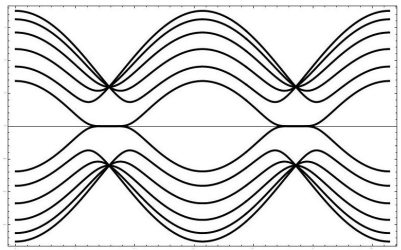
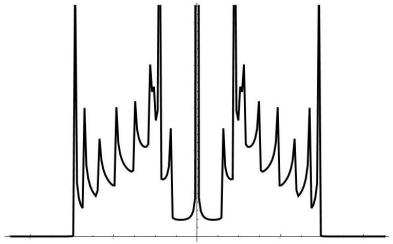
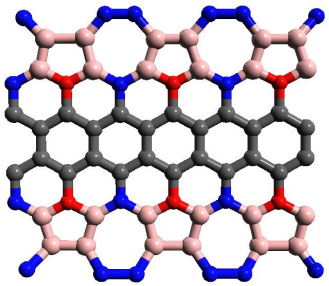
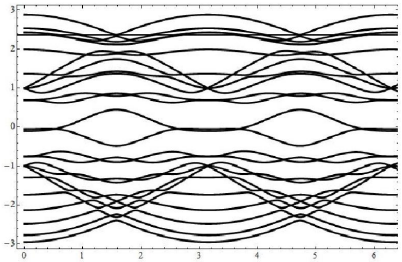
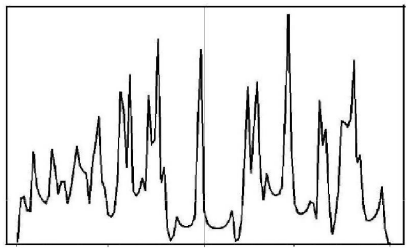
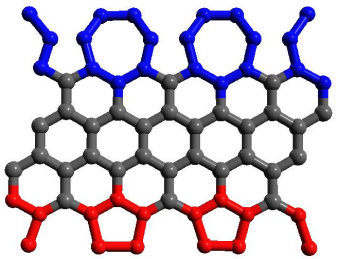
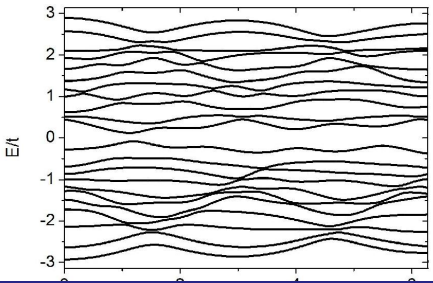
- in this way, the density of states shows around zero either a significant peak or the area with low presence of electrons [6]

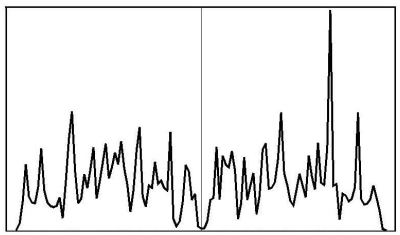




Electronic Properties of Graphene Nanoribbons in Magnetic Field

- the variations in the edge structure cause the variations in the electronic spectrum and density of states [7]:



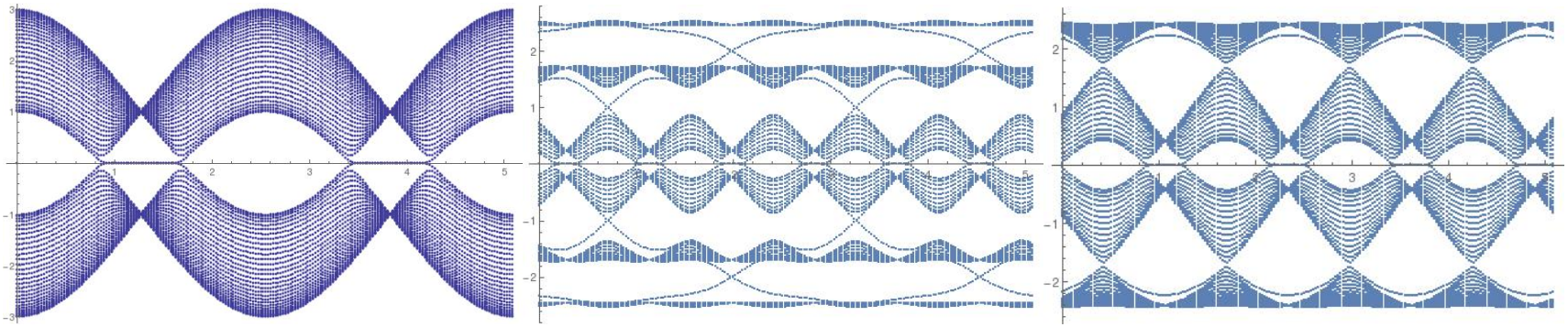
Electronic Properties of Graphene Nanoribbons in Magnetic Field

- in the presence of an uniform magnetic field, the corresponding Schrödinger equation has the form which is called the Harper equation [8,9]:

$$E\psi_i = \sum_{j,k} (te^{i\gamma_{ij}}\psi_j + t'e^{i\gamma_{ik}}\psi_k)$$

  - t, t' - the nearest and the next-nearest neighbor hopping integral
  - γ_{ij} - magnetic phase factor, it is proportional to the magnetic flux $f = p/q$, where p and q are mutual primes; different values of this flux significantly influence the form of the electronic spectrum which remains the same, but the size is changed

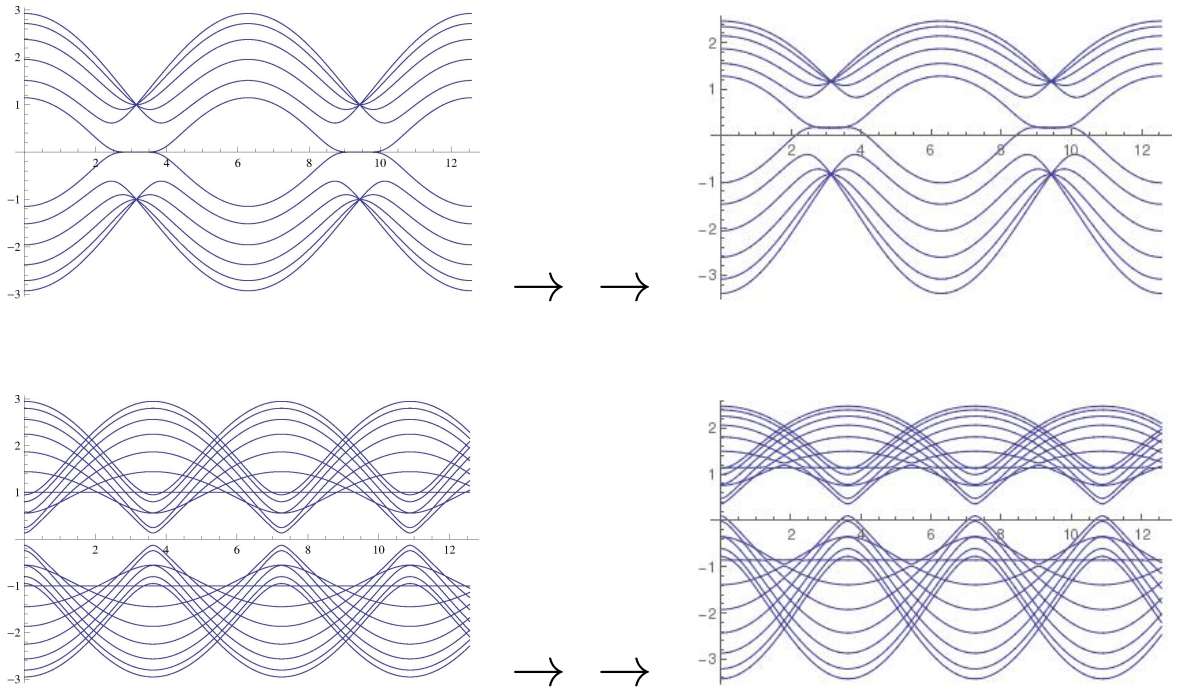
Electronic Properties of Graphene Nanoribbons in Magnetic Field



Electronic spectrum of zigzag nanoribbon for different values of the magnetic field given by the magnetic flux [10]: $f = 0$ (left), $f = 1/3$ (middle) and $f = 1/2$ (right).

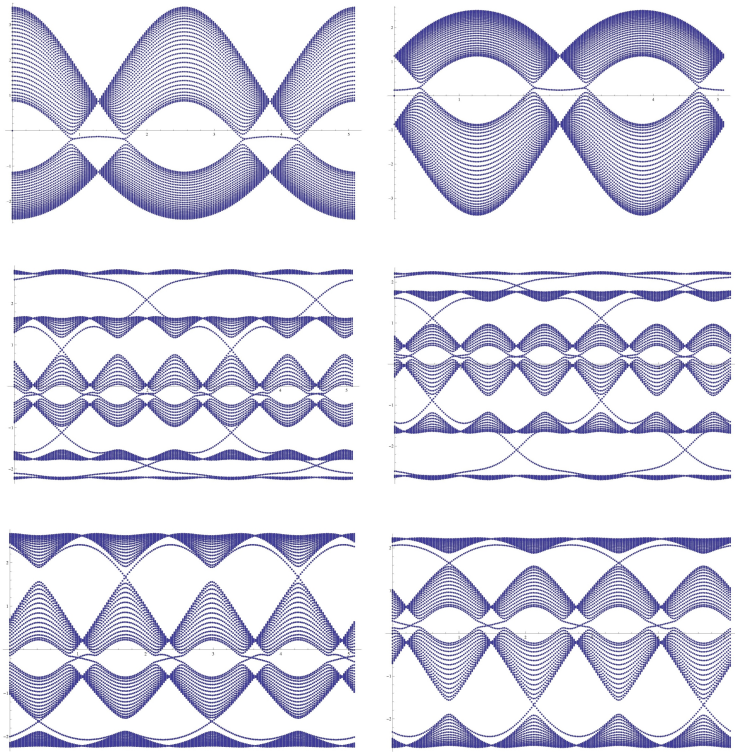
Electronic Properties of Graphene Nanoribbons in Magnetic Field

- up to now, we saw the results for the nearest-neighbor approximation; if we consider the inter-atomic interactions for higher distance, the following change of the electronic spectrum appears for the basic forms of zigzag and armchair nanoribbons:



Electronic Properties of Graphene Nanoribbons in Magnetic Field

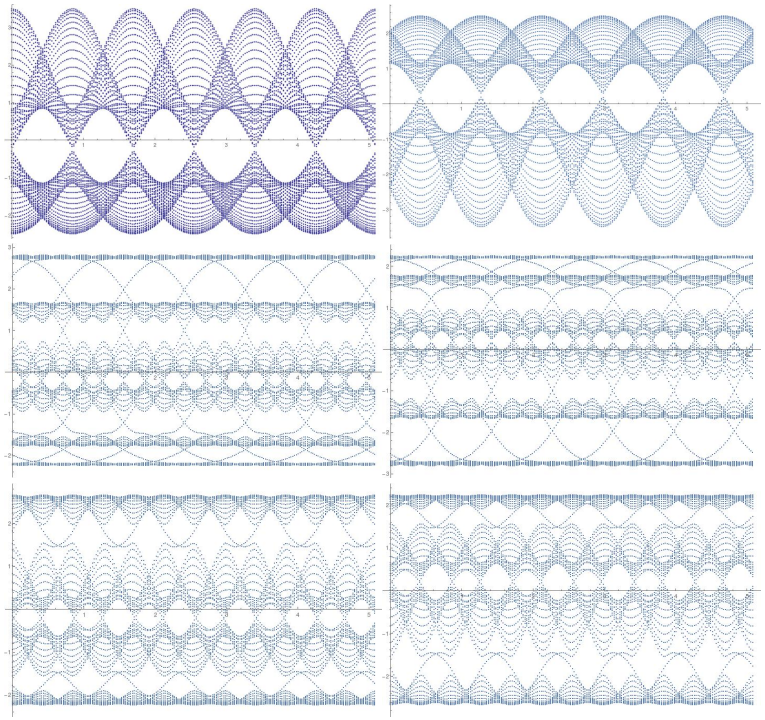
- in an adequate way, the electronic spectrum will be changed in the presence of the magnetic field:



Electronic spectrum of zigzag nanoribbons for different values of the magnetic flux: from up to down - $f = 0$ a $f = 3$, $f = 1/3$ a $f = 8/3$, $f = 1/2$ a $f = 5/2$.

Electronic Properties of Graphene Nanoribbons in Magnetic Field

- similarly, the same plots can be done for the armchair case:



Electronic spectrum of armchair nanoribbons for different values of the magnetic flux: from up to down - $f = 0$ a $f = 3$, $f = 1/3$ a $f = 8/3$, $f = 1/2$ a $f = 5/2$.

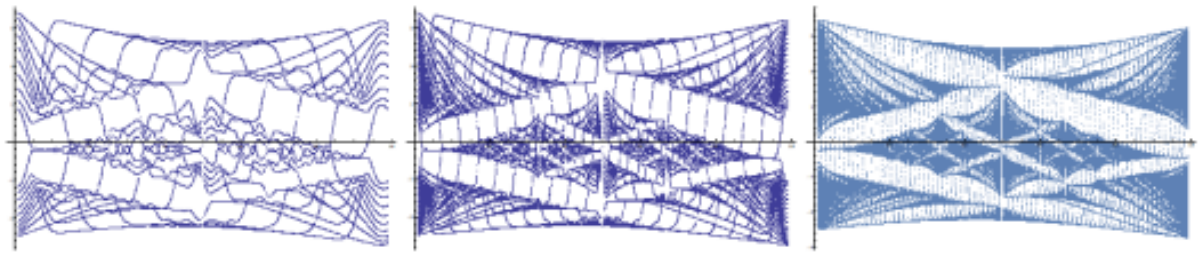
Electronic Properties of Graphene Nanoribbons in Magnetic Field

- the presented electronic spectra show an important aspect of the electronic structure: for a given value of q in the expression for magnetic flux ($f = p/q$), the resulting form of the electronic spectrum is q-times smaller than in the case when $f = 1$; as the consequence, if we would plot the energy dependence on the magnetic flux, the resulting graph would contain the *self-similar* parts; in other words, it would have the structure of fractal, here we speak about so-called *Hofstadter butterfly* [11]

Electronic Properties of Graphene Nanoribbons in Magnetic Field

- for the nearest-neighbor approximation, the dependence of the electronic spectrum on the magnetic flux is periodic with the length of period $f = 1$:

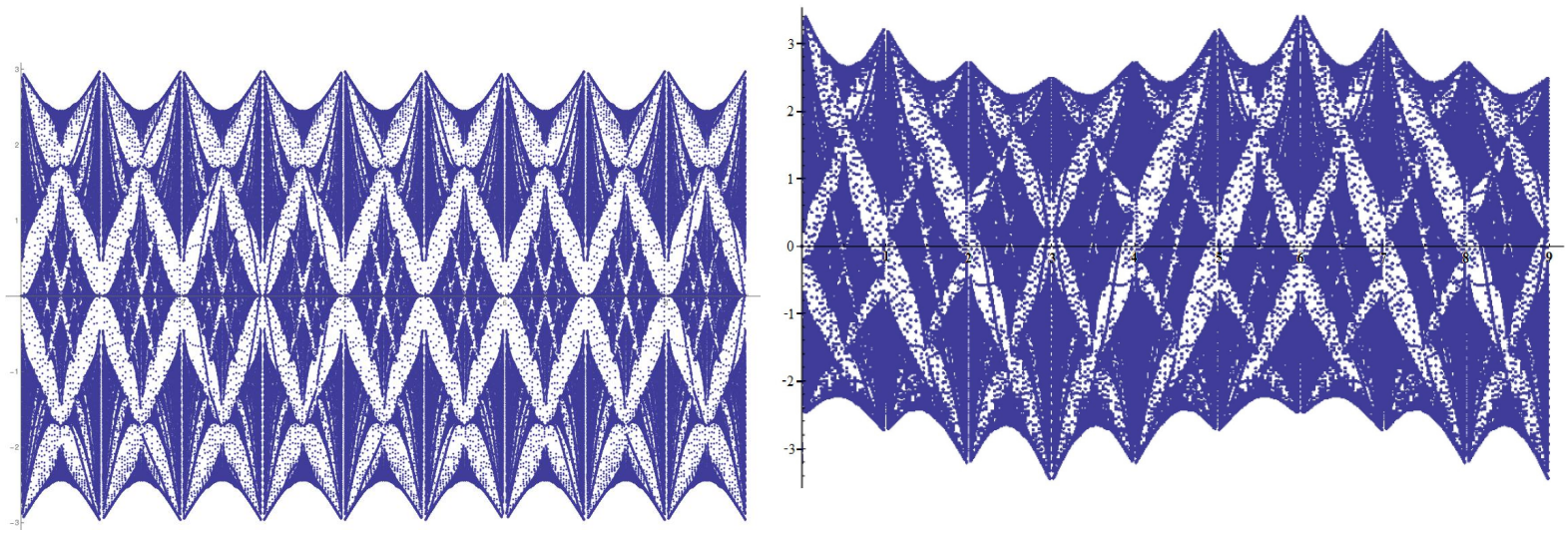
- for the case of next-nearest-neighbor approximation, the corresponding period is much longer (f=6) and that is why for the same interval of values, the corresponding plot is not symmetric:



the electronic spectrum depending on magnetic field for next-nearest-neighbor approximation and different widths of nanoribbon: 10 atoms (left), 20 atoms (middle) and 80 atoms (right)

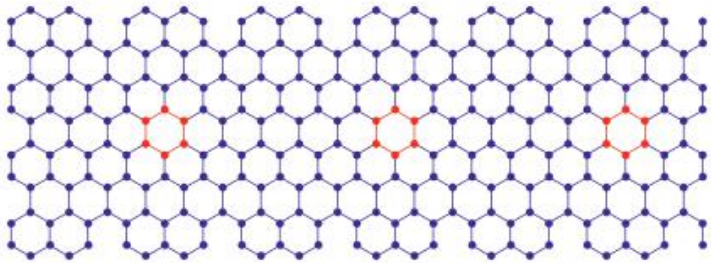
Electronic Properties of Graphene Nanoribbons in Magnetic Field

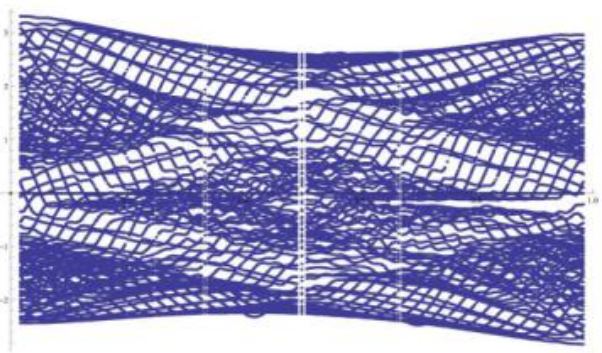
- in the interval of values $f \in (0, 6)$, the corresponding dependences for the nearest-neighbor and next-nearest-neighbor approximation have the following forms:

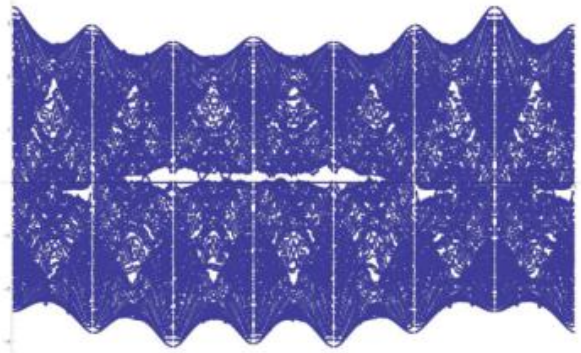


Electronic Properties of Graphene Nanoribbons in Magnetic Field

- here, we introduce variations of the zigzag nanoribbon together with the spectral dependence on the magnetic field (red atomic sites are excluded):







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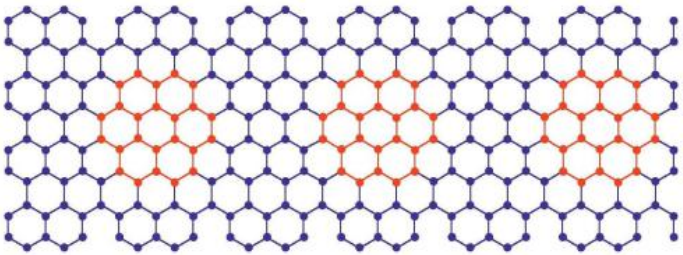

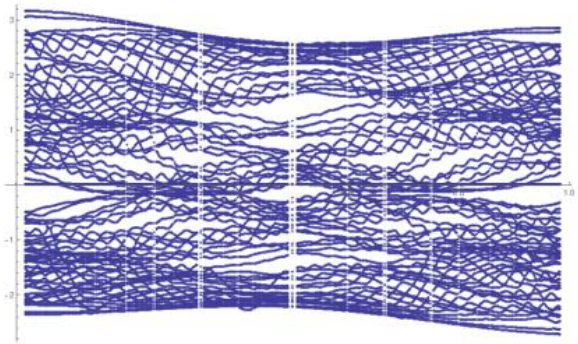

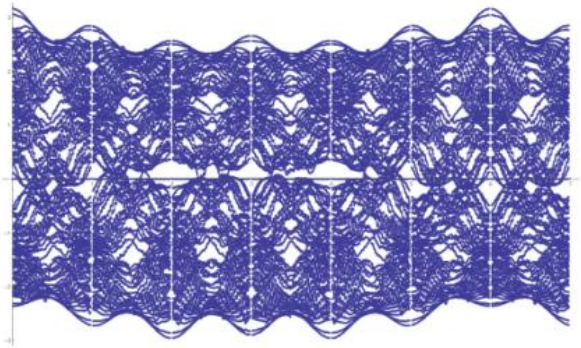

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Thank you for your attention