Electronic of 1D nanographite ribbons in modulated magnetic fields

1. Geometry
2. Tight-binding model
3. Electronic properties
   • transverse modulated magnetic field
   • longitudinal modulated magnetic field

4. summary

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Gemetric structures: 1D carbon nanoribbon

2D graphene sheet

\[ C_h = na_1 + ma_2 \]

- A atoms
- B atoms

Translation period: \( a \)
Translation period: \( 3b \)

- (a) zigzag edge
- (b) armchair edge

\( b = 1.42 \)
Experiments

I. Lithographically patterned GNRs

II. Cutting mechanically exfoliated graphenes

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FIG. 3. (Color online) STM images and a cross section near a monoatomic step with zigzag edge at the surface of ZYX ($T = 300$ K, in air, $I = 1.0$ nA, $V = 0.1$ V). (a) $30 \times 30$ nm$^2$ scan image. (b) Cross section profile along the arrow in (a). (c) $6 \times 6$ nm$^2$ scan image of the square region in (a). The dashed and dot-dashed lines show the edge and the atomic row of B-site atoms, respectively. The diamond and hexagon represent the $(\sqrt{3} \times \sqrt{3})R30^\circ$ supersstructure and honeycomb one.

FIG. 4. (Color online) STM images and a cross section near a monoatomic step with armchair edge at the ZYX surface ($T = 300$ K, in air, $I = 1.0$ nA, $V = 0.1$ V). (a) $30 \times 30$ nm$^2$ scan image. (b) Cross section profile along the arrow in (a). (c) $6 \times 6$ nm$^2$ scan image of the square region in (a). The dashed line, dot-dashed line, diamond, and hexagon represent the same meanings as in Fig. 3(c).
The tight-binding model

Eigenfunction: \[ \Psi = a_A \psi_A + a_B \psi_B \]

\[ \psi_A = \frac{1}{\sqrt{N}} \sum_{r_A} e^{i k \cdot r_A} \phi(r - r_A) \]

\[ \psi_B = \frac{1}{\sqrt{N}} \sum_{r_B} e^{i k \cdot r_B} \phi(r - r_B) \]

N \equiv \text{the number of A (B) atoms per unit cell}

Hamiltonian element:

\[ H_{AA} = H_{BB} = 0 \]

\[ H_{AB} = H_{BA}^* = e^{ik \cdot (r_B - r_A)} \langle \phi(r)|H|\phi(r - (r_B - r_A)) \rangle = -\gamma e^{ik \cdot (r_B - r_A)} \]

Sum to the nearest neighbors:

\[ H = \begin{bmatrix}
0 & H_{A,B_2} & 0 & 0 & 0 \\
H_{A,B_1} & 0 & H_{A,B_3} & 0 & 0 \\
0 & H_{A,B_2} & 0 & \ddots & 0 \\
0 & 0 & \ddots & 0 & H_{A_{N-1}B_N} \\
0 & 0 & 0 & H_{A_NB_N-1} & 0 \\
\end{bmatrix} \]

\[ \rightarrow H\Psi = \varepsilon\Psi \rightarrow \varepsilon = \]

\[ 2N \times 2N \]

2N atoms
Band Structures

Armchair ribbons

N=3I+2 (I an integer)  metal
Others  semiconductors

Zigzag ribbons

Zigzag ribbons with partial flat bands are all metals

PRB 54 17954 (1996)
• The partial flat bands can be understood as localized states near the zigzag edge.
• When the wave number deviates from $k = \pi$, the electron gradually penetrates towards the inner sites. Finally, the electron states completely extend at $k = 2 \pi / 3$.

The wavefunctions of the partial flat band

FIg 9. The charge density of the edge state at (a) $k = \pi$, (b) $k = 8\pi/9$, (c) $k = 7\pi/9$, and (d) $k = 2\pi/3$, where the radius of the circle means the magnitude of the charge density.
Spatially modulated magnetic along x-axis

\[ \mathbb{R}_B' = 2 \]

\[ \mathbf{R}_B' \equiv \frac{\text{field period length}}{\text{ribbon translation period}} \]
Bloch function in a magnetic field:

$$\Psi(k, r) = \frac{1}{\sqrt{N}} \sum_R e^{(ik \cdot R + \frac{G_R}{\phi_0} \phi(\gamma - R))}$$

Peierls phase:

$$\theta_R \equiv 2\pi \frac{G_R}{\phi_0} = \frac{2\pi}{\phi_0} \int_R A(l) \cdot dl; \quad \phi_0 = \frac{\hbar}{e} \quad \text{(flux quantum)}$$

Spatially modulated magnetic field:

$$B = B' \sin Kx \hat{z}; \quad K = \frac{2\pi}{3bR_{B'}}$$

$$A = (0, -\frac{B'}{K} \cos Kx, 0)$$
The x-dependence peierls phase:

\[ \theta_{i,j} = \frac{2\pi}{\phi_0} \int_i^j (0, -\frac{B'}{K} \cos Kx, 0) \cdot dl \]

\[ x_n \equiv \frac{b}{2} n ; \]

\[ \Phi' = \frac{3\sqrt{3}B' b^2}{2} \phi_0 \text{ (magnetic flux)} \]

\[ \begin{cases} 
\theta_1 = 0 \\
\theta_2 = \frac{3 \Phi' R_B'^2}{\pi^2} \cos \frac{\pi (n + \frac{1}{2})}{R_B'} \sin \frac{\pi}{6 R_B'} \\
\theta_3 = \frac{3 \Phi' R_B'^2}{\pi^2} \cos \frac{\pi (n - \frac{1}{6})}{R_B'} \sin \frac{\pi}{6 R_B'} 
\end{cases} \]
Band structures

- Linear bands become parabolic bands
- Complete flat band destroyed
- Leads to partial flat band
- Energy gap reduced

\[ I_x \equiv \text{periodical length}=a (3b) \] for zigzag (armchair) ribbon
- Metallic armchair ribbon open a band gap

- For zigzag ribbon, the highly degenerate states at $E = \gamma_0$ are destroyed, and all energy bands are oscillating parabolic bands.
The magnetic-flux-dependent energy gaps

- The size of band gap sensitive to the field period and amplitude
- Metal-semiconductor transition appears
Density of states

- Alters the peaks number, position and height
- Linear bands to parabolic bands induce square-root divergences
- Arising symmetric divergences
• The delta-function-like peak at $E_F=0$ in zigzag ribbon becomes lower as $R_B'$ grows.

• The plateau structure of metallic armchair ribbon at the Fermi level is opened a band gap.
Summary

• The transverse Modulated magnetic field modifies energy dispersions, alters subband spacings, adds band-edge states, changes band gap, and causes metal-semiconductor transitions.

• All the features are dominated by the field’s period, amplitude, and ribbon geometry.

• If the field’s period is large enough, the 1D energy bands would be transformed into 0D discrete states.
Spatially modulated magnetic field along y-axis

\[ \lambda = \frac{\text{field period length}}{\text{ribbon width}} \]
\[ \theta_1 = 0 \]

\[ \theta_2 = \frac{2}{3} \frac{\Phi_3}{\pi \lambda^2} \left( \frac{3}{2} N - 1 \right)^2 \cos \frac{\lambda \pi}{2} \left( \frac{6 n' - 1}{2} \right) \sin \frac{\lambda \pi}{2 \left( \frac{3}{2} N - 1 \right)} \]

\[ \theta_3 = -\frac{\Phi_4}{3 \pi \lambda^2} \left( \frac{3}{2} N - 1 \right)^2 \cos \frac{\lambda \pi}{2} \left( \frac{6 n' - 1}{2} \right) \sin \frac{\lambda \pi}{3 N - 2} \]

\[ \mathbf{A} = \left( \frac{B'}{K} \cos K y, 0 \right); \quad K = \lambda \frac{2\pi}{\left( \frac{3}{2} bN - b \right)} \]

\[ \theta_{i,j} = \frac{1}{\Phi_0} \int_i^j \mathbf{A} \cdot d\mathbf{l} \]

\[ y = 3bn'; \quad n' = 0, 1/2, 1, 3/2 \ldots \]
• N=600 armchair ribbon are all doubly degenerate parabolic bands, with band-edge states at $K_x=0$, and has a band gap.

• N=599 armchair ribbon has four-fold and two-fold degenerate states, and linear bands at the Fermi energy.
Band structures under magnetic fields

Uniform magnetic:
• Metal-semiconductor transition
• Partial flat subbands
• Wave function hits ribbon edge

Modulated magnetic field:
• Metal-semiconductor transition
• Oscillating subbands
• Wave function hits ribbon edge and magnetic field edge

“Magnetic and quantum confinements on electronic and optical properties of graphite ribbons”
Y. C. Huang, C. P. Chang, M. F. Lin
• The band edge of oscillating subbands touch the landau-level energy around $K_x = 0$
• More landau states appear than $\lambda = 1$
• The magneto-electronic wave function hits the magnetic field edge before the ribbon width
- The energy dispersions and state degeneracy are different between $K_x$ and $\bar{K}_x$ due to the asymmetric magnetic field on the ribbon width.
• As the $\lambda$ becomes small, the band structures are almost identical to the non-magnetic condition.

$\lambda = 1/2$
• The energy bands are almost identical to the N=600 case, except the states around $k_x=0$ at higher energy.

• At large $K_x$, electrons only view one edge of the ribbon and are independent of the ribbon width.
• For N=600 armchair, the large $\lambda$ needs, the small magnetic field is to derive the metal-semiconductor transition.

• Only a very weak magnetic field could open an energy of N=599 armchair.

• The wider the ribbon is, the easier to close the band gap.
Density of states

- Alters the peaks number, position and height.
- At $\lambda = 2$, the first two peaks position are very close to the uniform magnetic field.
- At $\lambda = 1/2$, band gap is opened.
• The modulated magnetic field would modify energy dispersions, state degeneracy and cause metal-semiconductor transitions.

• Under the modulated magnetic field, the electrons confined by the ribbon width and the field edge, different field period would have great influence on electronic properties.

• The uniform magnetic field would lead to complete flat bands (landau levels) as the filed strength is large enough. On the other hand, under the modulated magnetic field, the energy bands always disperse versus wavenumber.
Thank you~