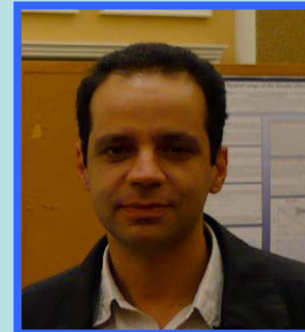


Zigzag graphene ribbons and coupled chains

Nancy Sandler
Ohio University

In collaboration with: Medhi Zarea



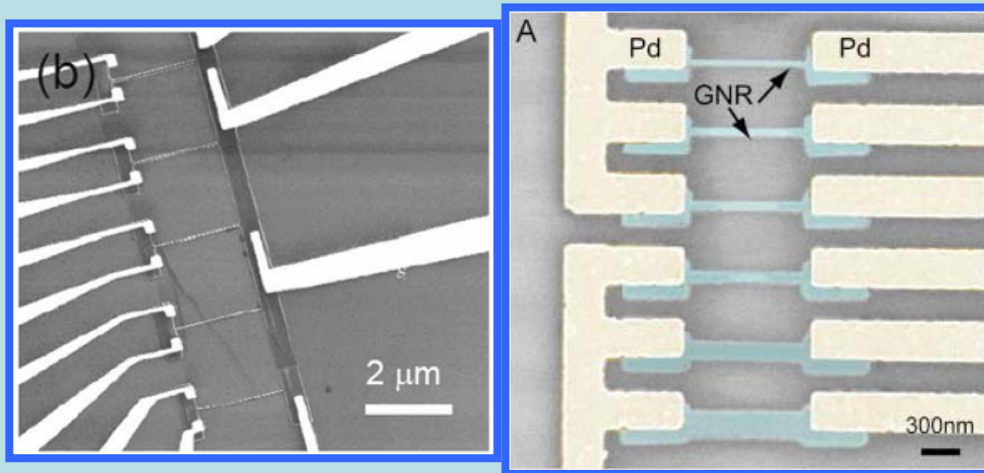
April 2009

Graphene Week KITP



Ribbons: some methods of fabrication

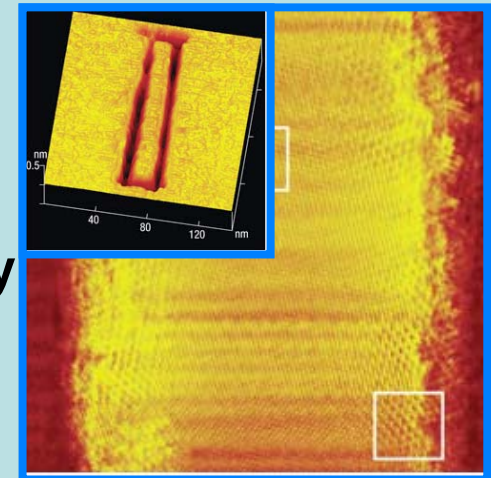
Lithographic patterning



Kim PRL (2007)

Avouris Physica E (2007)

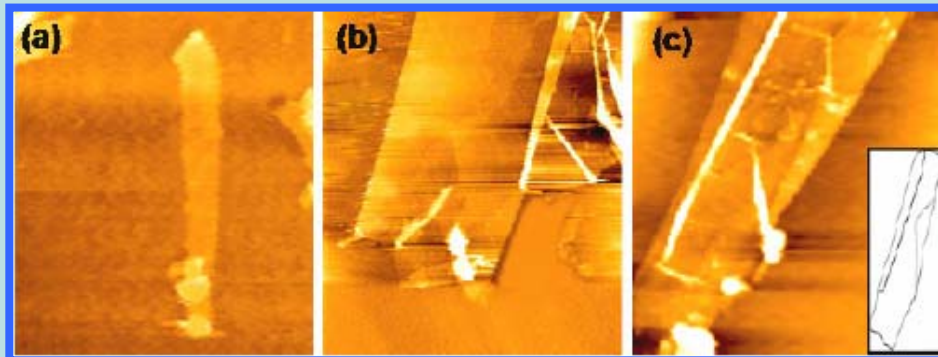
STM lithography



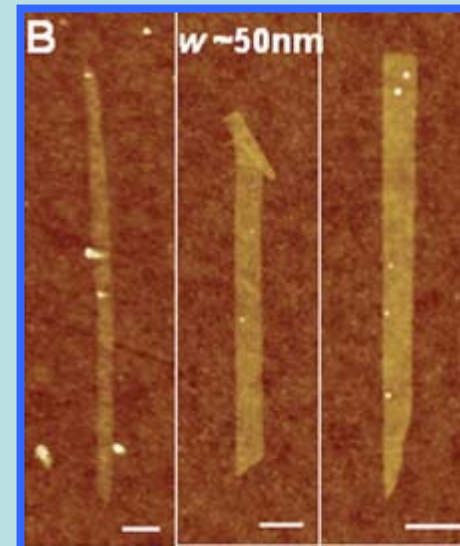
Biro Nat. Nanot. (2008)

Exfoliated graphite in solution

Electrostatic deposition with gas



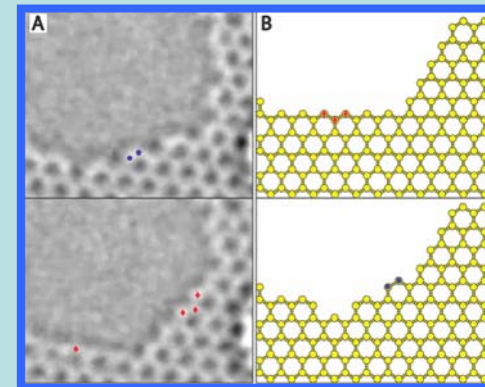
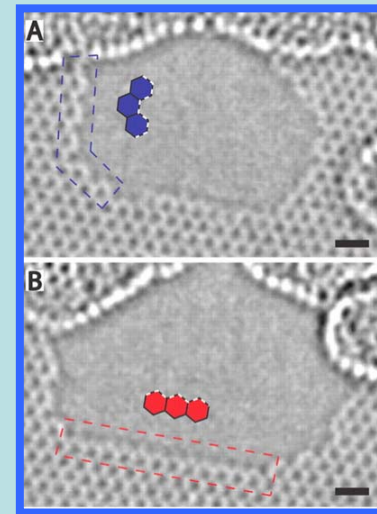
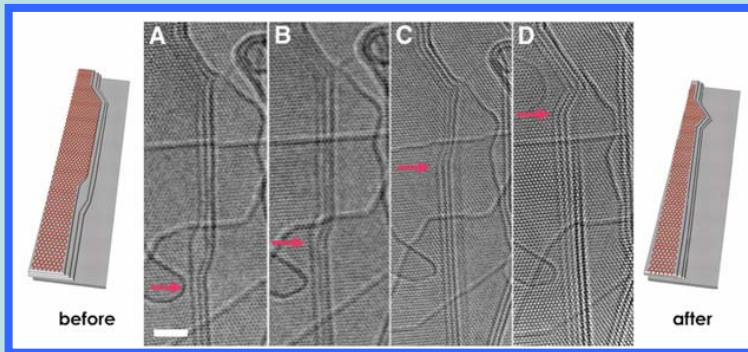
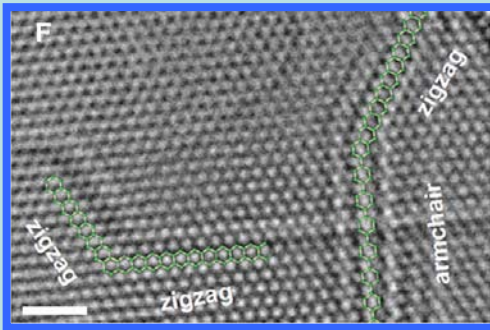
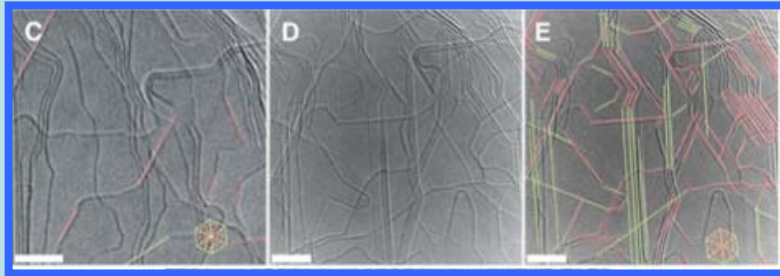
Wu Nanotechnology (2009)



Dai
Science (2008)

Edges... Last two: cleaner edges of armchair or zigzag

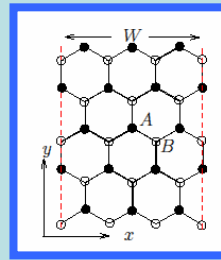
Also: edge reconstruction



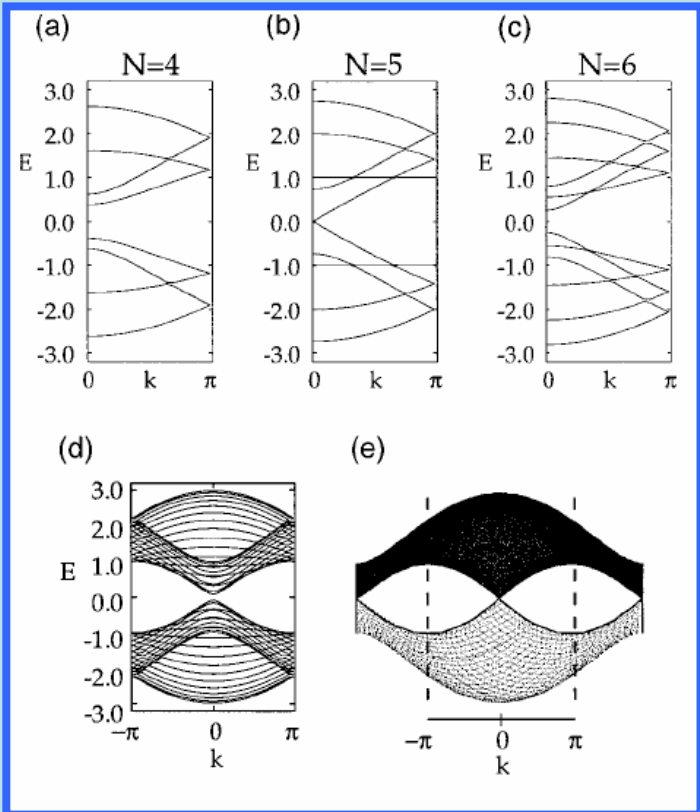
Crommie Science (2009)

Dresselhaus Science (2009)

Armchair ribbons



- Long-range Coulomb

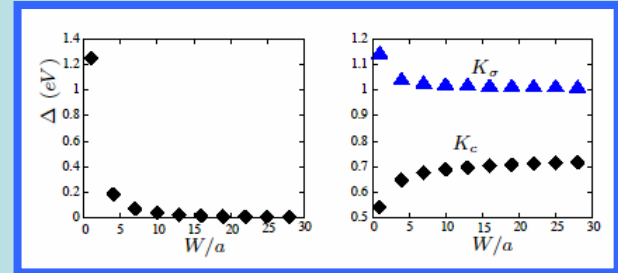


TB + Hard
Wall BC=
Wavefunctions
Effective 1d
Coulomb +
Bosonization

$$\Delta \propto \frac{1}{W}$$

- Intrinsic Spin-orbit

$$\psi_{\pm}^s = N e^{\pm s \gamma_0 (x - W/2)} \sin\left(\frac{4\pi x}{3a}\right) \frac{e^{ik_y y}}{\sqrt{2L}} \begin{pmatrix} 1 \\ \pm i \end{pmatrix}$$



Nakada et al, PRB (1996)

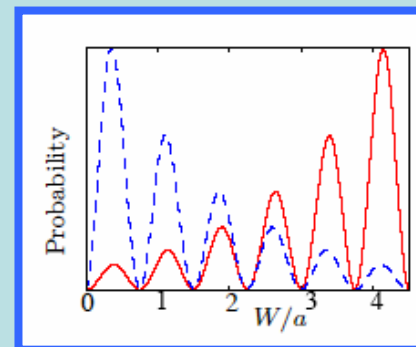
K. Nakada et al. PRB (1996)

M. Fujita et al. J. Phys. Soc. Jpn. (1996)

T. Hikiyama et al. PRB (2003)

L. Brey and H. Fertig PRB (2006)

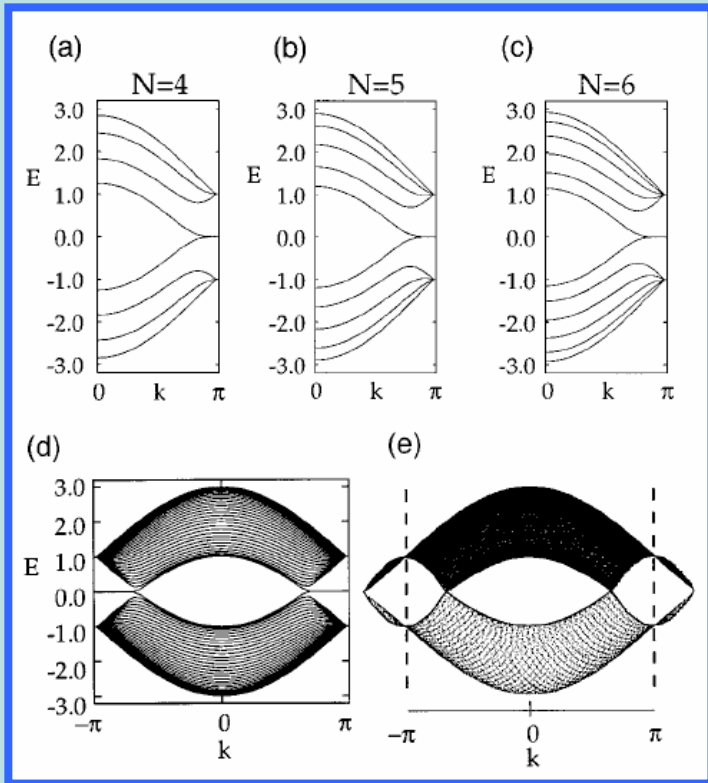
M. Zarea, N.S. PRL (2007)



$\gamma_0 \approx t'$
 \pm : left/right movers
 s : spin

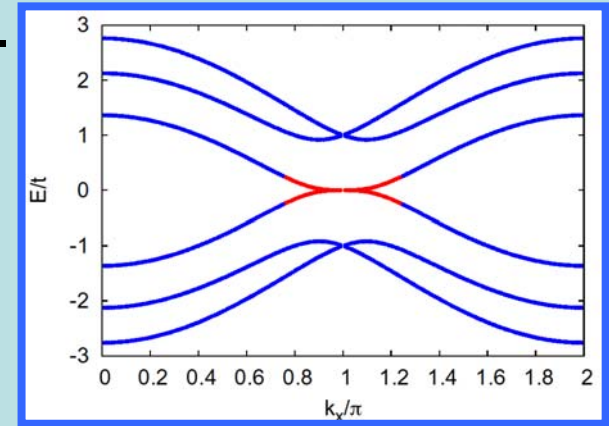
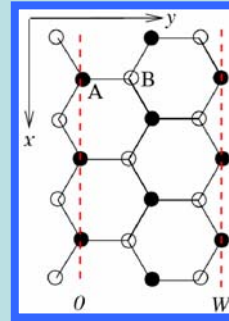
**Spin-filtered
edge states.**

Zigzag Ribbons



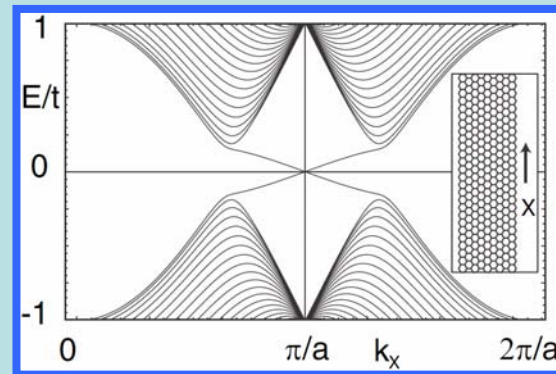
Nakada et al, PRB (1996)

TB + Hard Wall= Band-structure and wave- functions.



$$\psi = e^{ik_x x} \left[\begin{pmatrix} 1 \\ e^{-k_y W} \end{pmatrix} e^{ik_y y} - \begin{pmatrix} 1 \\ e^{k_y W} \end{pmatrix} e^{-ik_y y} \right]$$

• Intrinsic spin orbit



C. Kane and E. Mele PRL (2005)

H. Min et al. PRB (2006)

J. Boettger et al. PRB (2006)

D. Huertas-Hernando et al PRB (2006)

- Gap opens: insulating bulk
- Spin-filtered edge states

Quantum Spin Hall Phase

K. Nakada et al. PRB (1996)

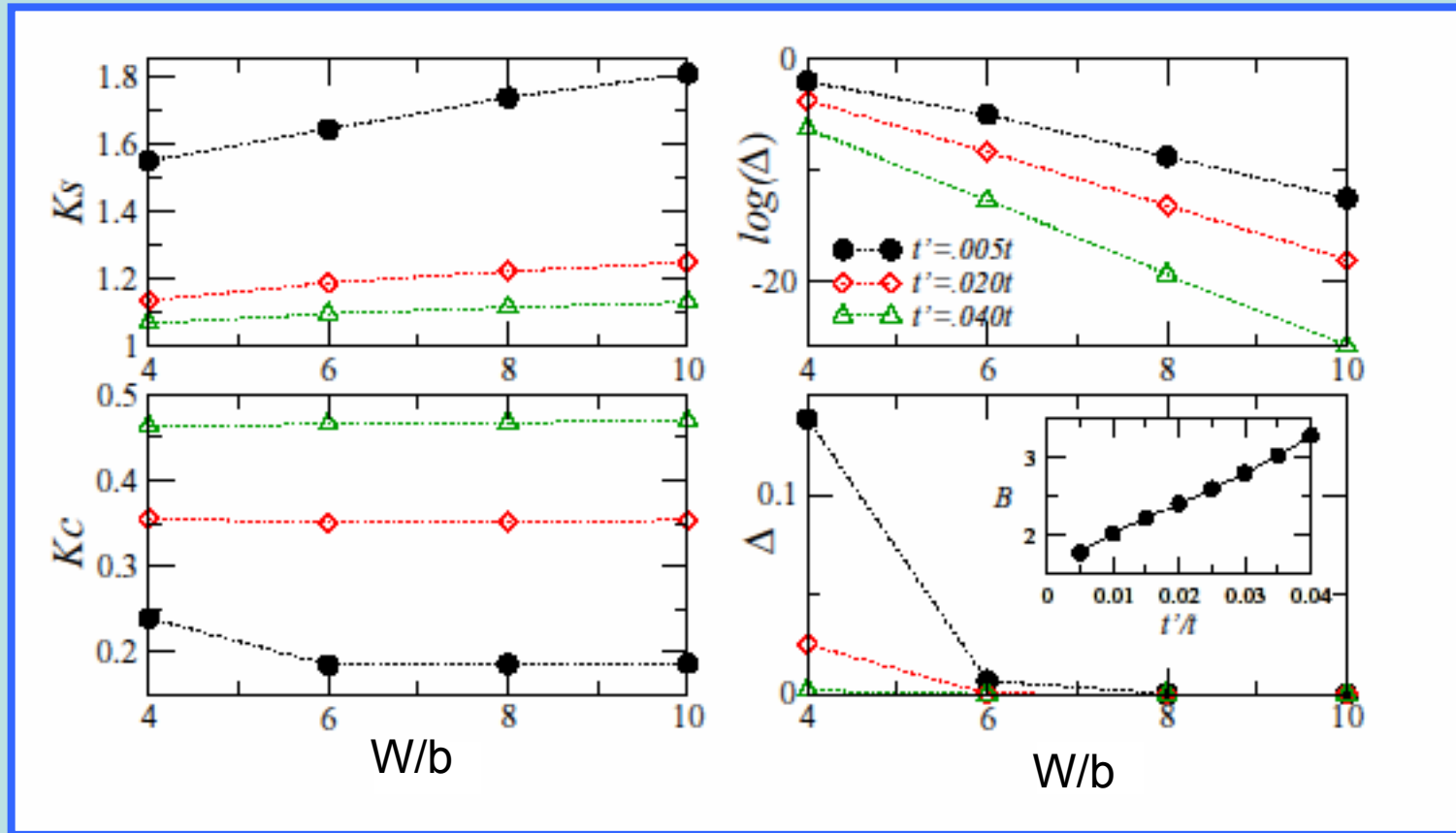
M. Fujita et al. J. Phys. Soc. Jpn. (1996)

T. Hikiyama et al. PRB (2003)

L. Brey and H. Fertig PRB (2006)

**What about Coulomb
interactions?**

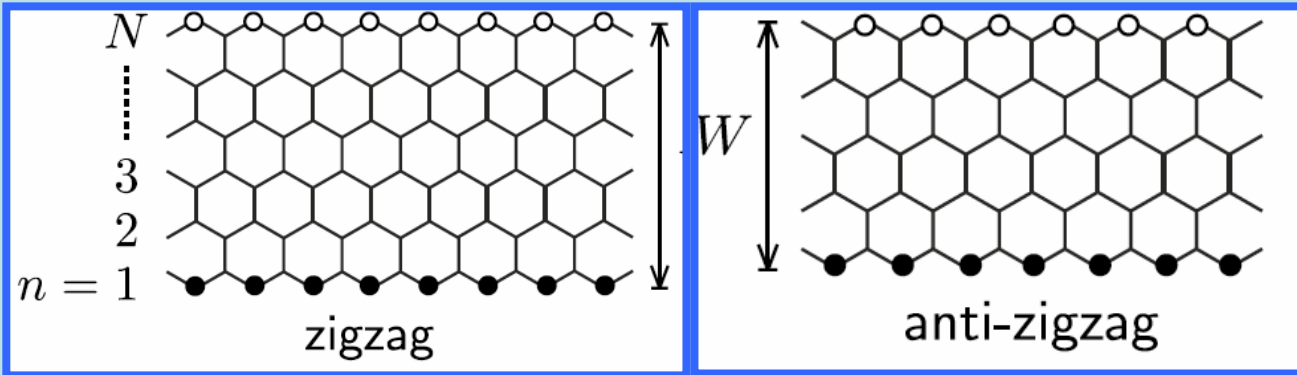
With I-SO interaction and bosonization



**Increasing
magnetic order
($K_s > 1$)**

$$\Delta \propto e^{-BW}$$

Even-Odd Feature:



Hikihara et al PRB (2003)
 Kohmoto and Hasegawa PRB (2007)
 Akhmerov et al PRB (2008)
 Li et al PRL (2008)
 Yao et al PRL (2009)

TB + Hard Wall BC = Wavefunctions finite system

$$\psi_{\pm} = C e^{ik_x x} \begin{pmatrix} \sin k_y (y + W/2) \\ \pm \sin[k_y (y - W/2) - \beta] \end{pmatrix}$$

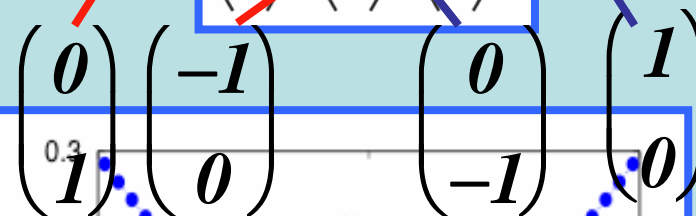
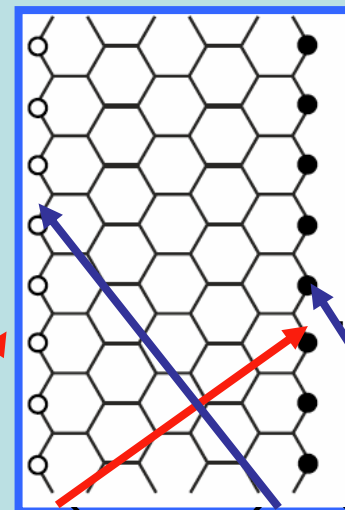
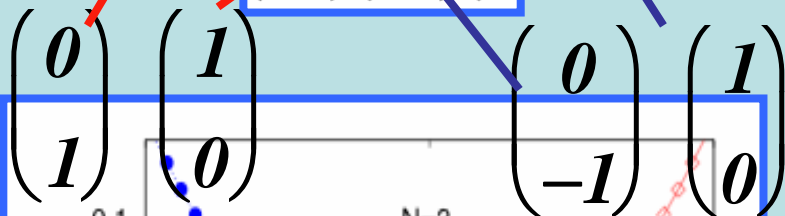
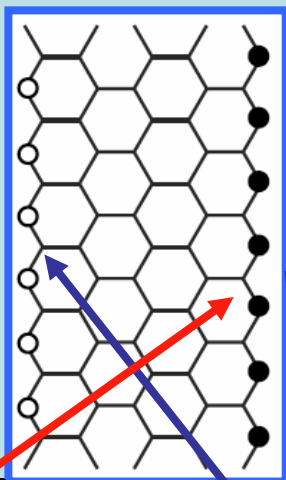
$$k_x a > \pi \quad \beta = 0 \quad k_y = iq$$

$$k_x a < \pi \quad \beta = \pi N \quad k_y = iq - \pi$$

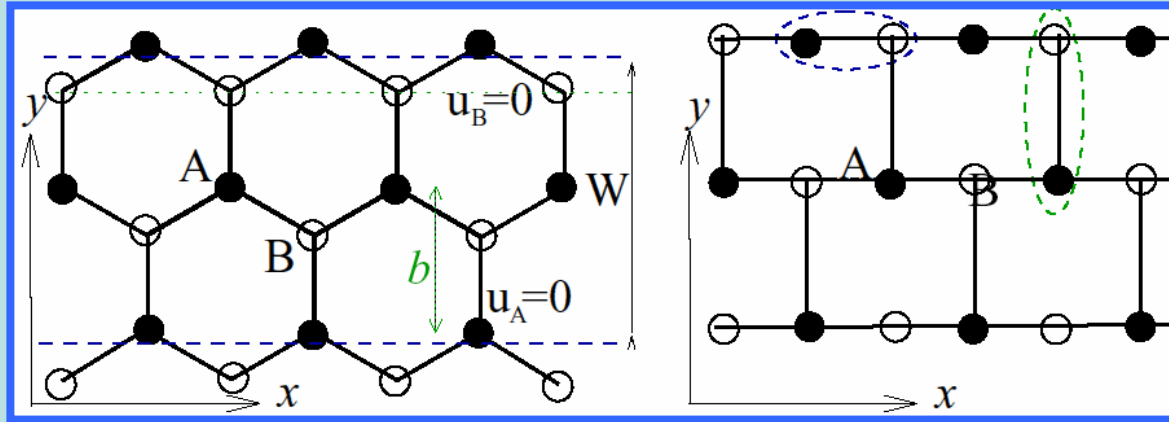
Could it be **so** important???

Near band center:

$$E \approx \pm t_{\perp} \left(\frac{tk}{t_{\perp}} \right)^N$$



Coupled chains:



$$H_N = \sum_{n=1}^N H_n + t_{\perp} H' \quad \leftarrow \text{Coupling between chains}$$

$$H_n = \int dx [t c_{A_n}^+(x)(c_{B_n}(x) + c_{B_n}(x-a)) + h.c.]$$

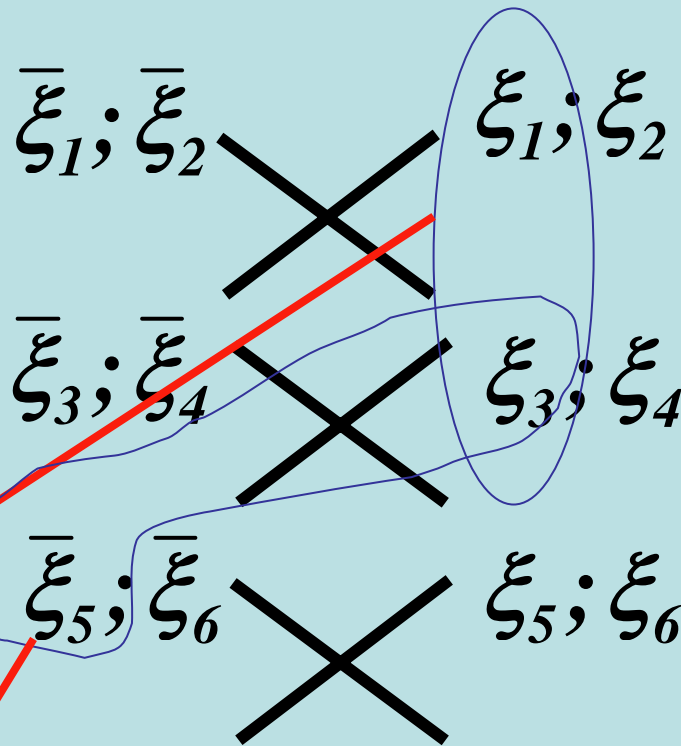
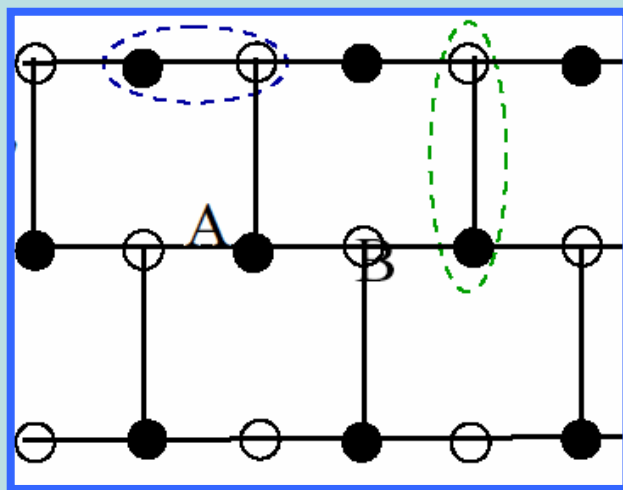
Right and Left moving operators: even and odd sites

$$H_{n,0} = -iv(R_n^+ \partial_x R_n - L_n^+ \partial_x L_n)$$

Introduce Majorana representation

$$R_n = (\xi_{2n-1} + i\xi_{2n})/\sqrt{2}$$

$$L_n = (\bar{\xi}_{2n-1} + i\bar{\xi}_{2n})/\sqrt{2}$$

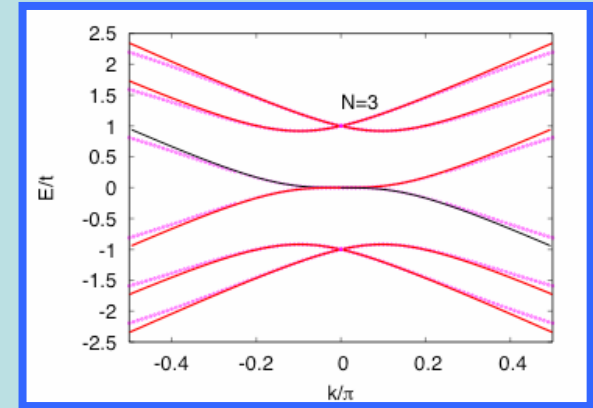
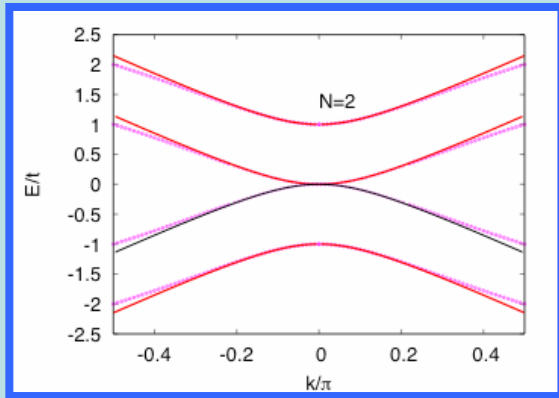


$$H_0 = \sum_{n=1}^{2N} iv (\xi_n \partial_x \xi_n - \bar{\xi}_n \partial_x \bar{\xi}_n)$$

$$H' = \sum_{n=1}^{2N-2} ih (\xi_n \xi_{n+2} - \bar{\xi}_n \bar{\xi}_{n+2}) + im (\xi_n \bar{\xi}_{n+2} - \bar{\xi}_n \xi_{n+2})$$

$$h = m = \frac{t}{2} = \frac{t_{\perp}}{2}$$

Hamiltonian: solved recursively

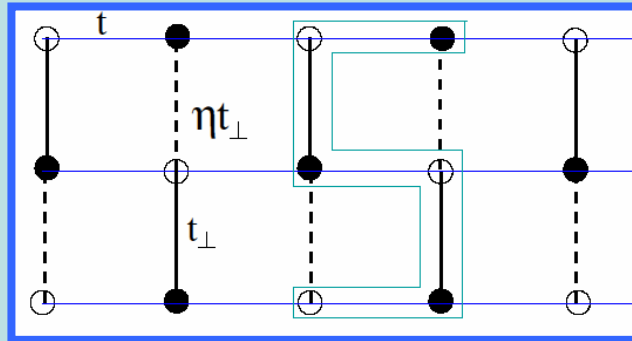


Can the model be generalized?

$$h \neq m \Rightarrow t \neq t_{\perp}$$

$$h = \frac{t_{\perp}}{2} (1 + \eta)$$

$$m = \frac{t_{\perp}}{2} (1 - \eta)$$

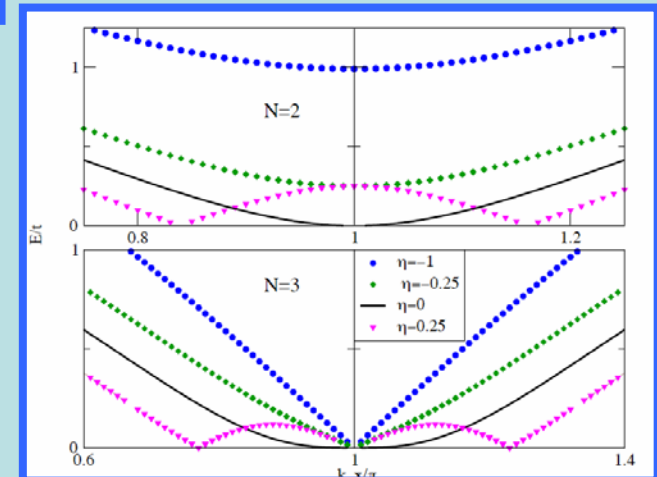


Square: $\eta = 1$
Graphene: $\eta = 0$
 π -Flux: $\eta = -1$

Affleck and Marston PRB (1988)
 Ludwig et al PRB (1994)

Band structure:

$$E = \pm \sqrt{\left(t \cos \frac{k_x a}{2} + 2h \cos k_y b \right)^2 + 4m^2 \sin^2 k_y b}$$



Rashba interactions?

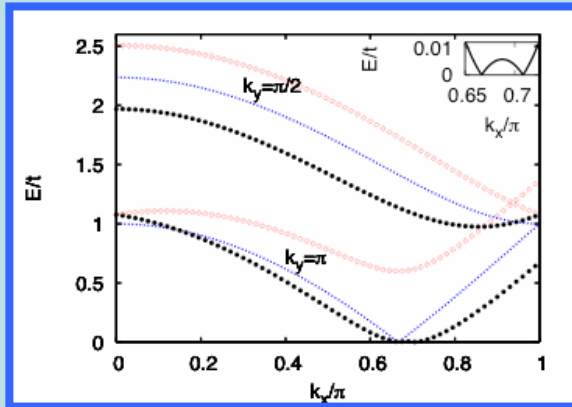
$$H_R = \sum_{\langle ij \rangle} ic_i^+ (\vec{u}_{ij} \cdot \sigma) c_j + h.c.$$

$$\vec{u}_{ij} = -\frac{\lambda_R}{d} \hat{z} \times \vec{\delta}_{ij}$$

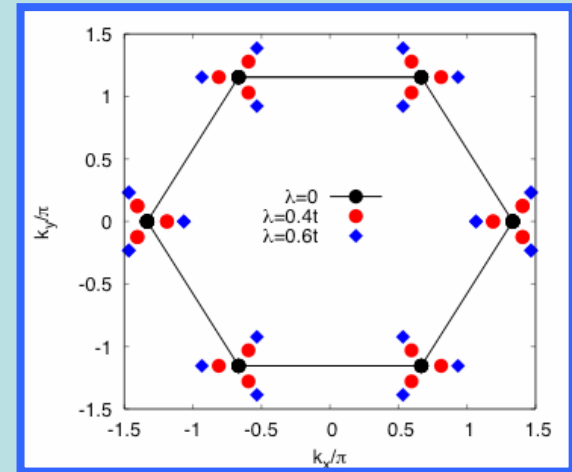
$$H = \begin{pmatrix} 0 & \varphi_0 & 0 & i\varphi_+ \\ \bar{\varphi}_0 & 0 & -i\bar{\varphi}_- & 0 \\ 0 & i\varphi_- & 0 & \varphi_0 \\ -i\bar{\varphi}_+ & 0 & \bar{\varphi}_0 & 0 \end{pmatrix}$$

$$\Psi = \begin{pmatrix} u_{A\uparrow} \\ u_{B\uparrow} \\ u_{A\downarrow} \\ u_{B\downarrow} \end{pmatrix}$$

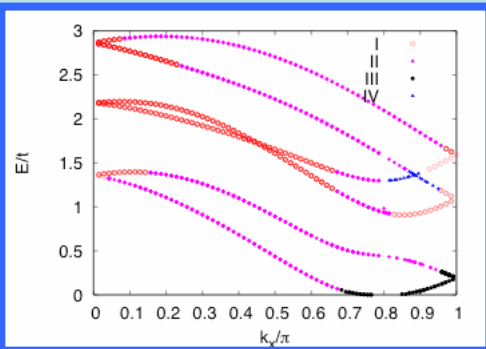
Bulk:



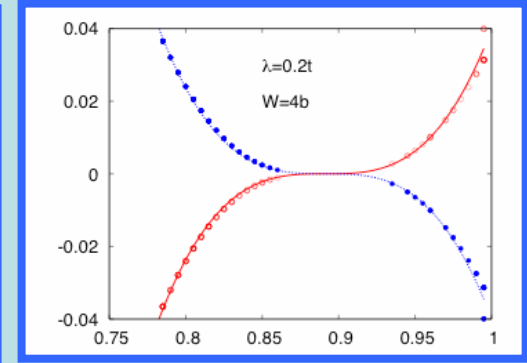
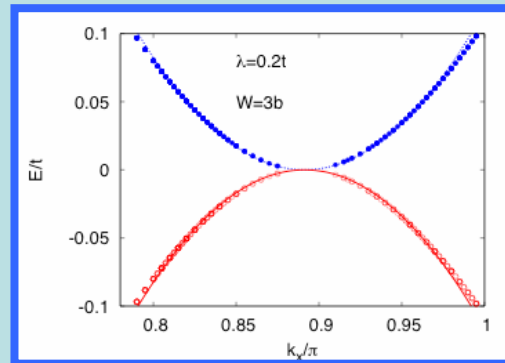
New Dirac points!



Zigzag ribbons:



Even-odd feature:



Relation to Quantum Spin Chains:

N= 2 ZGR \Leftrightarrow Anisotropic 2 coupled Spin 1/2 chains

$$H = t \sum_i \vec{S}_{1i} \cdot \vec{S}_{1j} + t_{\perp} S_{1i}^z \cdot S_{2j}^z$$

N= 3 ZGR \Leftrightarrow Anisotropic biquadratic Spin 1 chain with in plane B

Tsvelik PRB (1990)

Shelton et al PRB (1996)

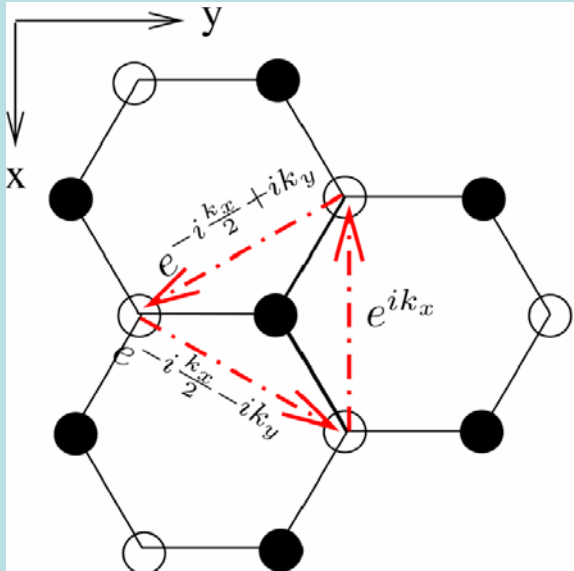
Advantages:

- Chemical potential $\xi_1 \xi_2$ (gap on chain)
- Second neighbor hopping = chemical potential
- Intrinsic spin-orbit (gap for even N) $t' (\xi_1 \bar{\xi}_3 + \bar{\xi}_1 \xi_3)$
- Staggered sublattice potential (gap for all N)
- Electron-electron interactions
- ...

Conclusions

- Zigzag ribbons: 'peculiar' edge states
- Mapping to coupled chains: metal or insulator as N changes
- Many lattices share similar properties
- Connections to Quantum Spin Chains.

The symmetries of graphene allow for: **the intrinsic spin-orbit interaction.**



$$H_{\uparrow} = \begin{pmatrix} \gamma & \Phi \\ \overline{\Phi} & -\gamma \end{pmatrix}$$

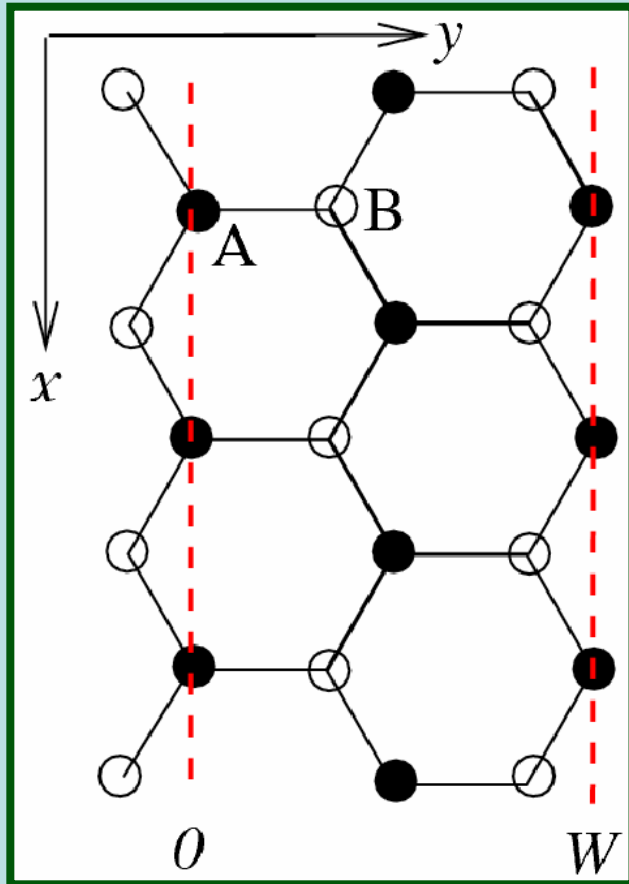
$$H_{\downarrow} = \begin{pmatrix} -\gamma & \Phi \\ \overline{\Phi} & \gamma \end{pmatrix}$$

$$\gamma = 2t' \left[\sin(k_x a) - 2 \sin(k_x a / 2) \cos(k_y b) \right]$$

$$E = \sqrt{|\Phi|^2 + \gamma^2}$$

C. Kane and E. Mele PRL 95 226801 (2005)
 H. Min et al. PRB 74, 165310 (2006)
 J. Boettger et al. PRB 75, 121402(R) (2006)

Zigzag ribbons: tight-binding and hard-wall boundary conditions



Wavefunction:

$$\psi = e^{ik_x x} \left[\begin{pmatrix} 1 \\ e^{-k_y W} \end{pmatrix} e^{ik_y y} - \begin{pmatrix} 1 \\ e^{k_y W} \end{pmatrix} e^{-ik_y y} \right]$$

$$k_y = k_y(W, k_x)$$

$$\tan \left[k_y \left(W - \frac{1}{2} \right) \right] = \frac{1 - 2 \cos \left(\frac{k_x}{2} \right)}{1 + 2 \cos \left(\frac{k_x}{2} \right)} \tan \left(\frac{k_y}{2} \right)$$

K. Nakada et al. PRB 54, 17954 (1996)

M. Fujita et al. J. Phys. Soc. Jpn. 65, 1920 (1996)

T. Hikihara et al. PRB 68, 035432 (2003)

L. Brey and H. Fertig PRB 73, 235411 (2006)