Graphene nanoflakes with defective edge terminations:

Tight-binding spectra (as a function of magnetic field), topological effects, and 1D quantum behavior

I. Romanosvky, C. Yannouleas, U. Landman

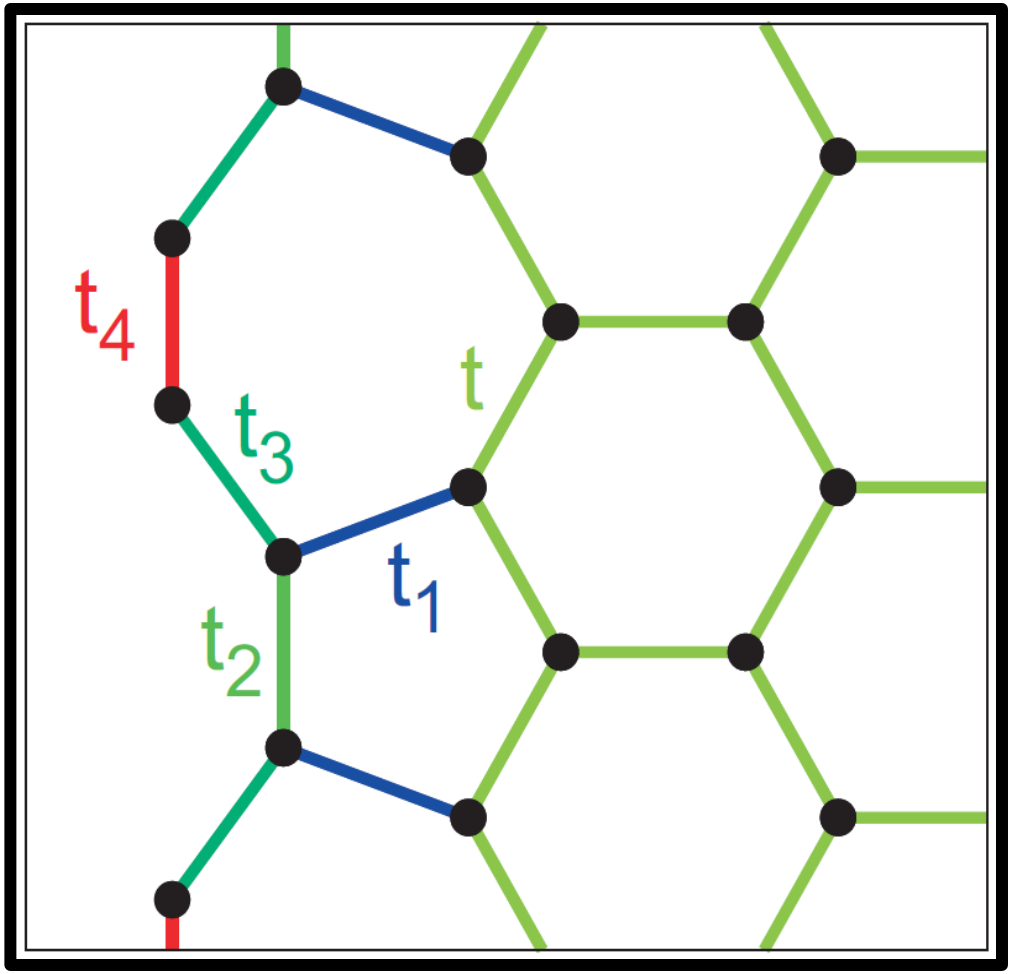
School of Physics
Georgia Institute of Technology

Phys. Rev. B **86,** 165440 (2012)

APS March 2013

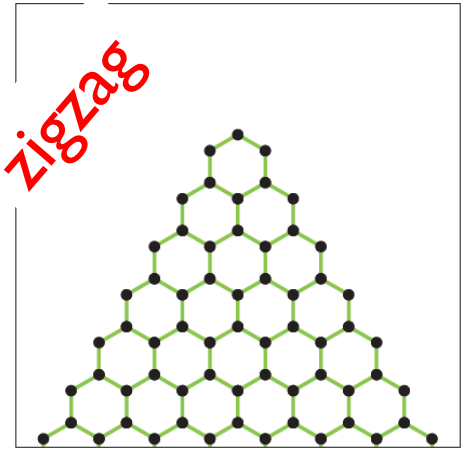
Supported by the U.S. DOE (FG05-86ER45234)

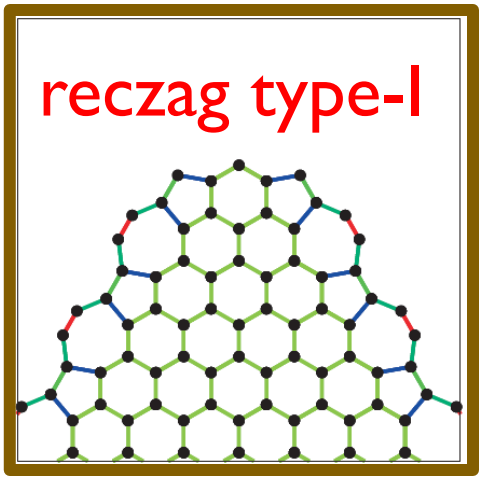
Reconstructed zigzag edge (reczag)

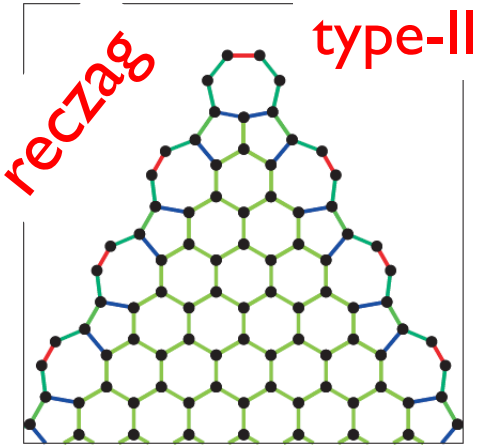


pentagon-heptagon

triangle/ corners







TIGHT-BINDING (TB) METHOD

$$H_{\mathrm{TB}} = -\sum_{<i,j>} \tilde{t}_{ij} c_i^{\dagger} c_j + h.c.,$$

nearest neighbor

$$\tilde{t}_{ij} = t_{ij} \exp\left(\frac{ie}{\hbar c} \int_{\mathbf{r}_i}^{\mathbf{r}_j} d\mathbf{s} \cdot \mathbf{A}(\mathbf{r})\right)$$

2.7 eV

Peierls factor

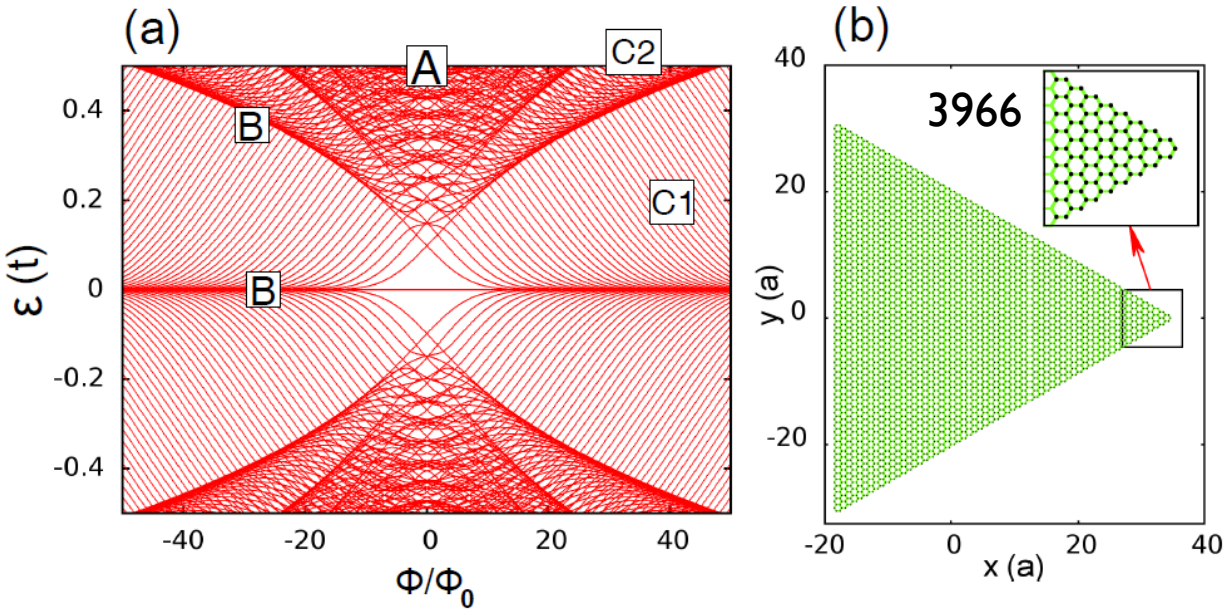
(Vector potential, magnetic field B)

$$M(\Phi) = -S \frac{dE_{\mathrm{tot}}}{d\Phi},$$

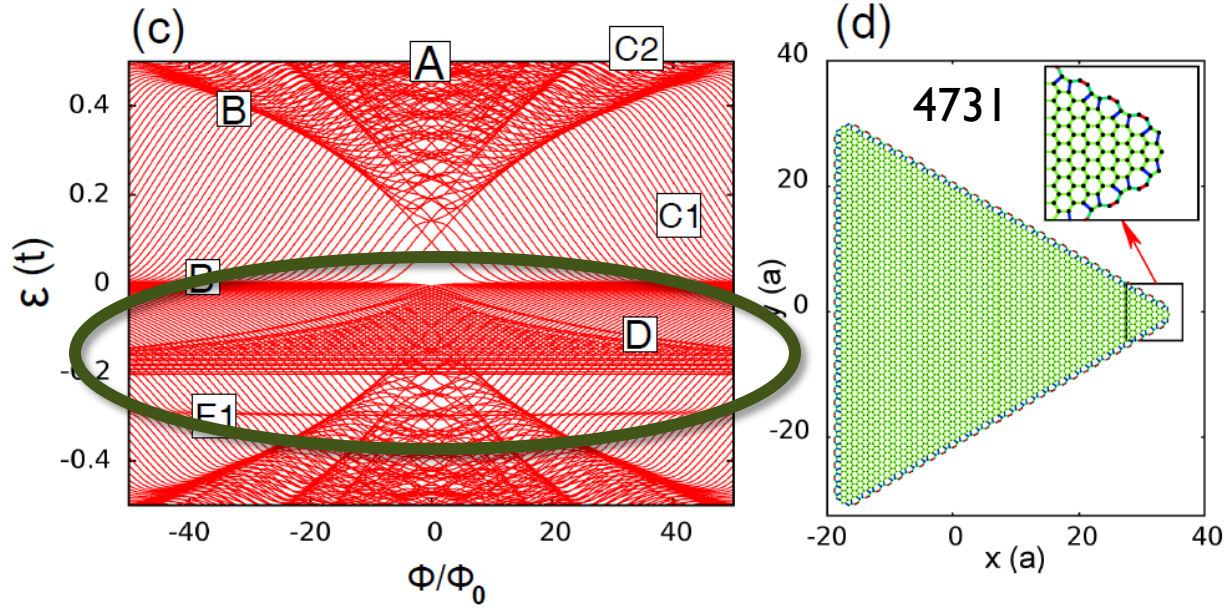
$$E_{\mathrm{tot}}(\Phi) = \sum_{i,\sigma}^{\mathrm{occ}} \varepsilon_i(\Phi)$$

TB spectrum triangle

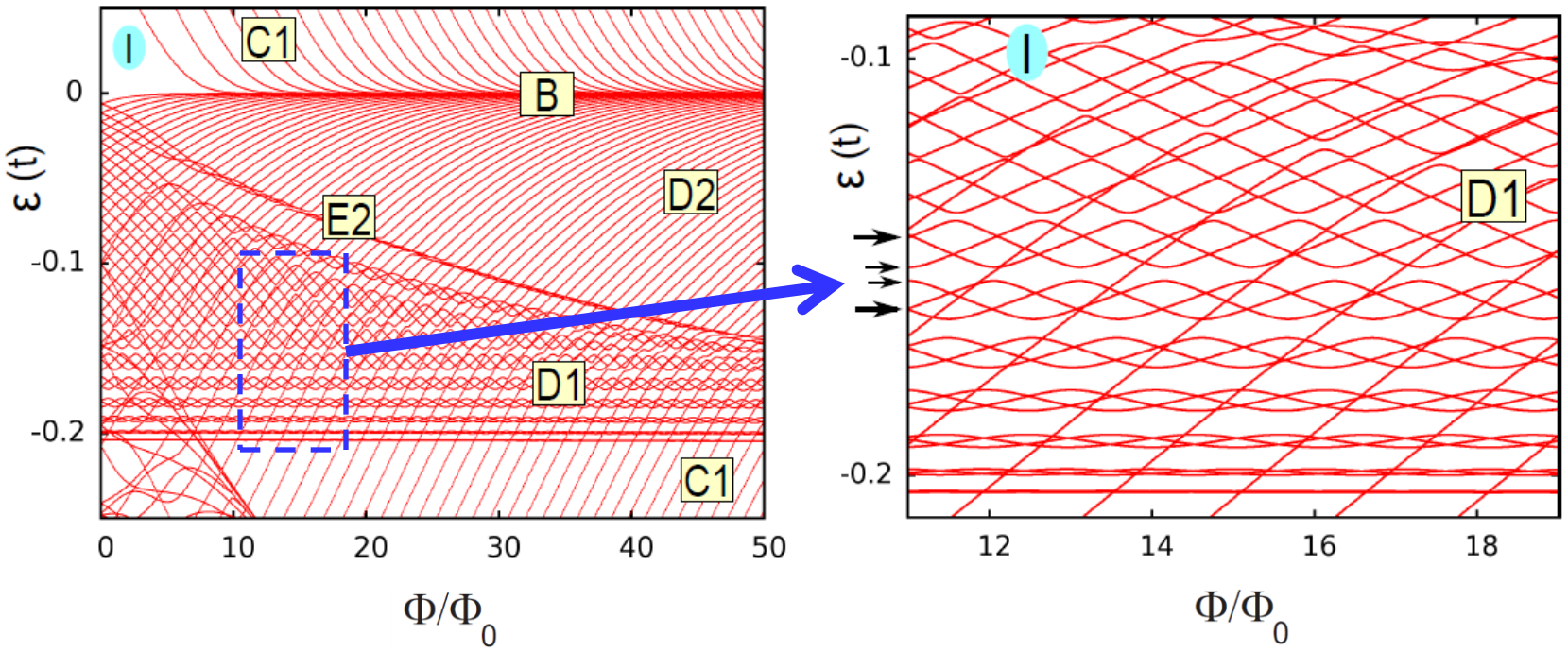
zigzag edge



reczag edge



Reczag TB spectrum details (region D1)



C1, D2: Halperin-type edge states (IQHE)

D1: Three-fold braid bands, 1D quantum wire around the trigonal flake

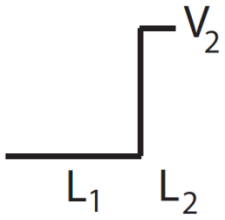
Modeling of reczag quantum ring:
Kronig-Penney model (nonrelativistic)

$$-\frac{1}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi(x)=E(x)\psi(x)$$

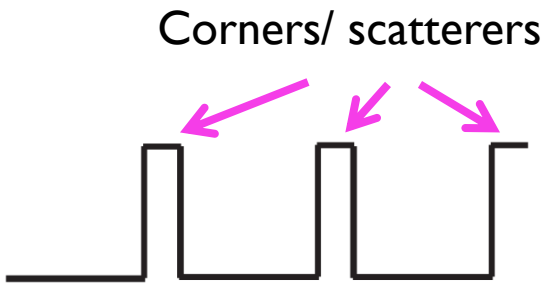
Schroedinger eq.

constant mass

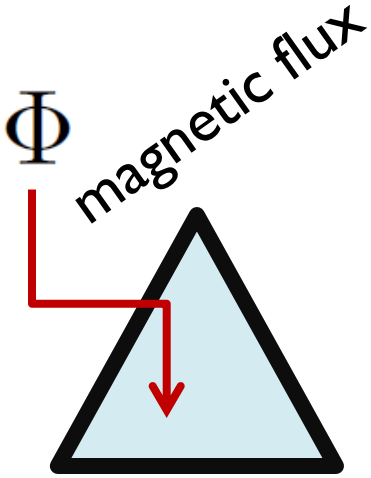
potential



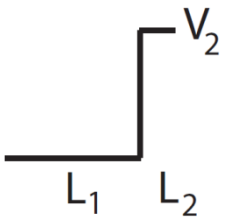
One side/ 2 regions



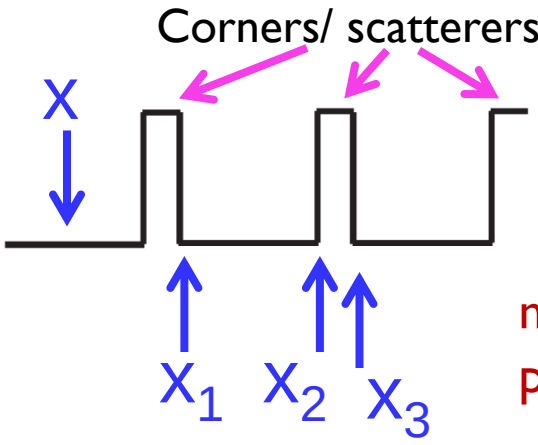
Triangle/ 3 sides/ 6 regions



One side/ 2 regions



Triangle/ 3 sides/ 6 regions



Transfer matrices

Basic

$$\mathbf{W}_K(x) = \begin{pmatrix} e^{iKx} & e^{-iKx} \\ iKe^{iKx} & -iKe^{-iKx} \end{pmatrix}$$

$$K^2 = \frac{2m(E-V)^2}{\hbar^2}$$

$$\mathbf{M}_K(x_1, x_2) = \mathbf{W}_K(x_2)\mathbf{W}_K^{-1}(x_1)$$

region

$$\mathbf{T_s} = \mathbf{M}_1\mathbf{M}_2$$

side

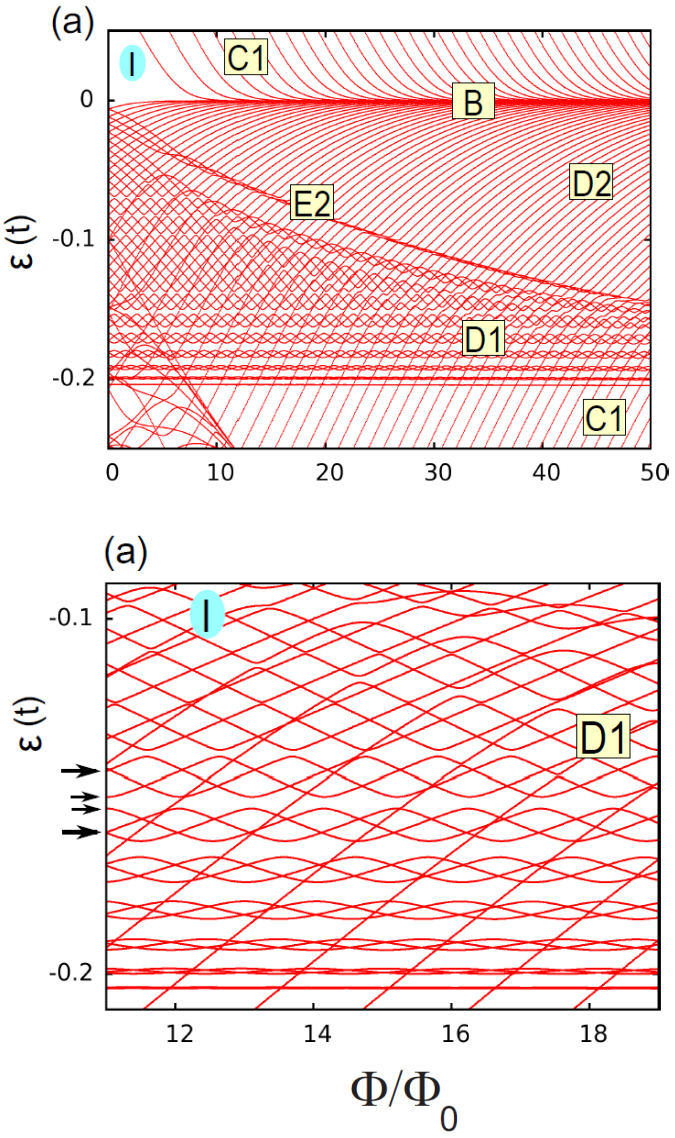
$$\mathbf{T} = \mathbf{T_s}^3$$

triangle

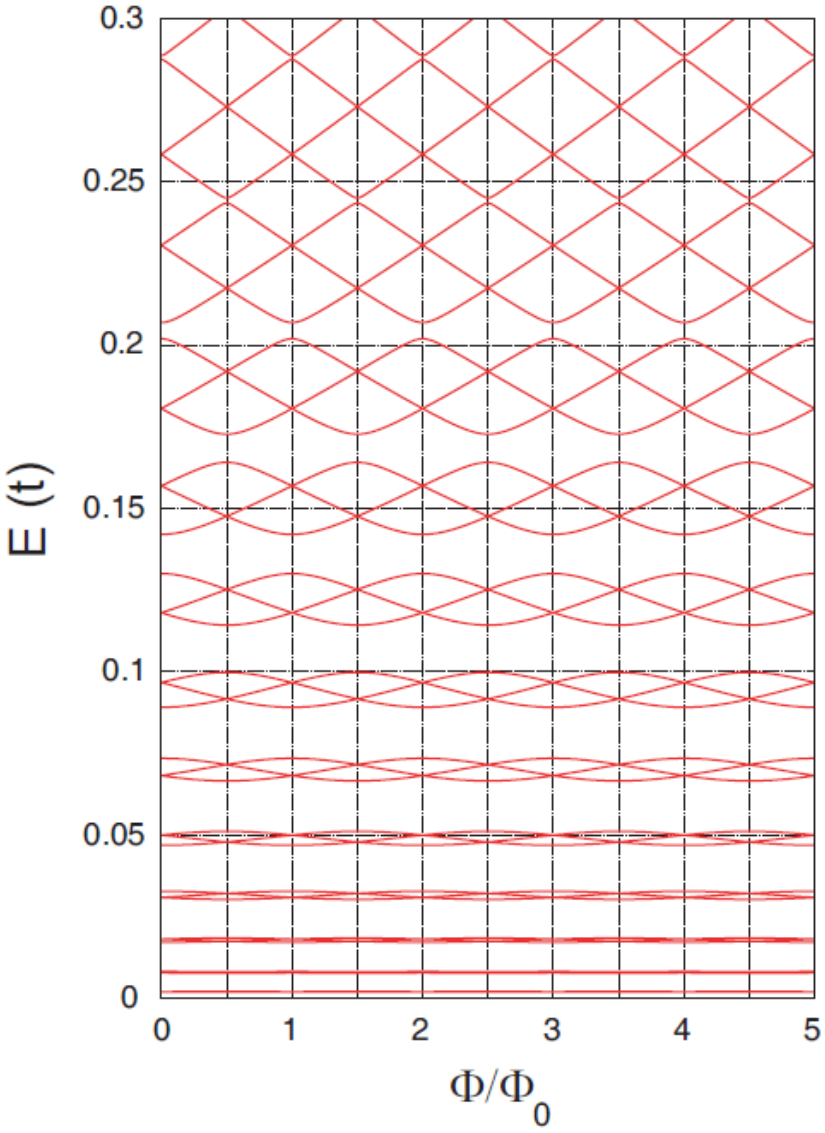
Virtual magnetic-field superlattice

$$\cos(2\pi\Phi/\Phi_0) = \mathrm{Tr}[\mathbf{T}(E)]/2$$

TB spectrum for reczag trigonal flake



1D Kronig-Penney model (nonrelativistic/ free-electron mass)



Conclusions

1) The spectra (as a function of B) of trigonal graphene nanoflakes with reczag edges do not exhibit particle-hole symmetry

2) New features appear compared to nanoflakes with zigzag edges

3) A prominent feature is the formation of threefold braid bands; they are explained by a (nonrelativistic) 1D Kronig-Penney superlattice model

4) The reczag edge behaves like a 1D quantum wire forming a nonrelativistic ring around the trigonal nanoflake

5) The threefold braid bands cannot be reproduced with the continuous Dirac-Weyl model