Graphene nanoflakes with defective edge terminations:
Tight-binding spectra (as a function of magnetic field),
topological effects, and 1D quantum behavior

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APS March 2013
Supported by the U.S. DOE (FG05-86ER45234)
Reconstructed zigzag edge (reczag)
TIGHT-BINDING (TB) METHOD

\[ H_{TB} = - \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j + h.c., \]

nearest neighbor

\[ \tilde{t}_{ij} = t_{ij} \exp \left( \frac{ie}{\hbar c} \int_{r_i}^{r_j} ds \cdot A(r) \right) \]

2.7 eV

Peierls factor

(Vector potential, magnetic field B)

\[ M(\Phi) = -S \frac{dE_{tot}}{d\Phi}, \quad E_{tot}(\Phi) = \sum_{i,\sigma}^{\text{occ}} \varepsilon_i(\Phi) \]
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)

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

- Schrödinger eq.
- Potential
- Constant mass

One side/ 2 regions

Triangle/ 3 sides/ 6 regions

Corners/ scatterers
Transfer matrices

Basic

\[ W_K(x) = \begin{pmatrix} e^{iKx} & e^{-iKx} \\ iKe^{iKx} & -iKe^{-iKx} \end{pmatrix} \]

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

\[ M_K(x_1, x_2) = W_K(x_2)W_K^{-1}(x_1) \]

region

Basic

Virtual magnetic-field superlattice

\[ \cos\left(\frac{2\pi \Phi}{\Phi_0}\right) = \text{Tr}[T(E)]/2 \]
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