Manipulating Dirac Physics with Mesoscopics in Graphene

Herb Fertig, Indiana University

I. Introduction: Quantized States of Graphene Ribbons
II. Transport Through Junctions and Polygons
III. "Effective Time-Reversal Symmetry Breaking" in Quantum Rings
IV. Periodic Potentials: Emergent Dirac Points
V. Summary

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A.P. Iyengar, Tianhuan Luo (Indiana)

Funding: NSF

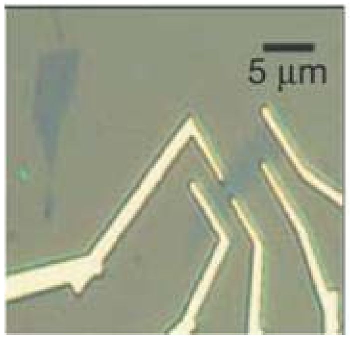
I. Introduction

• To what extent can we manipulate the electronic properties of graphene by selective cutting and/or application of potentials at very short length scales?

• New ideas for integrated circuit technology

Metallic conductivity $\Longrightarrow$ low power dissipation, higher frequency operation than traditional semiconductors

High thermal conductivity $\Longrightarrow$ cooling less challenging

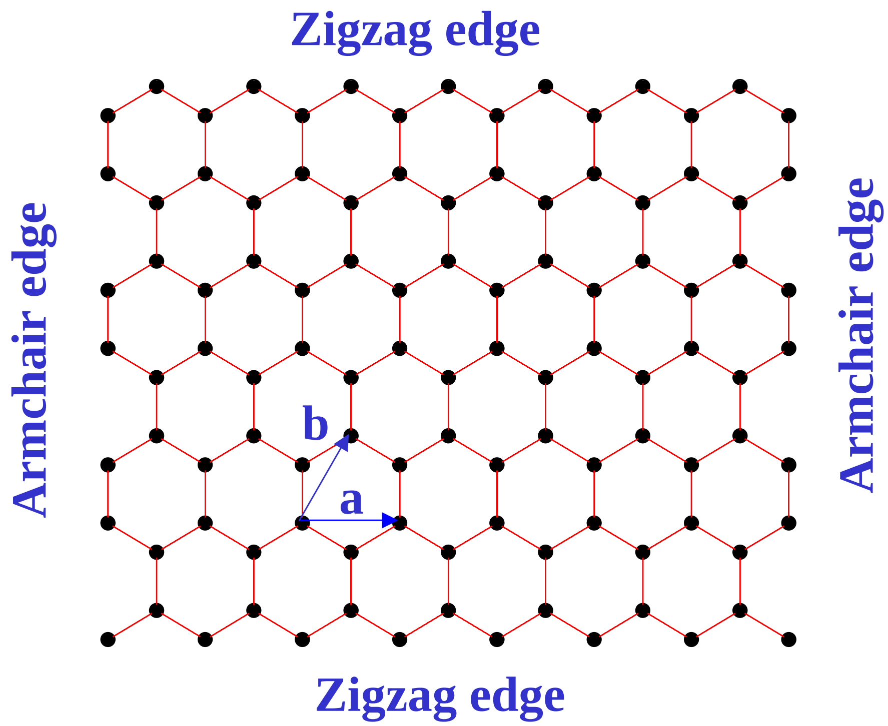


Kim Group
Nature 2005

Geim Group
Nature 2005

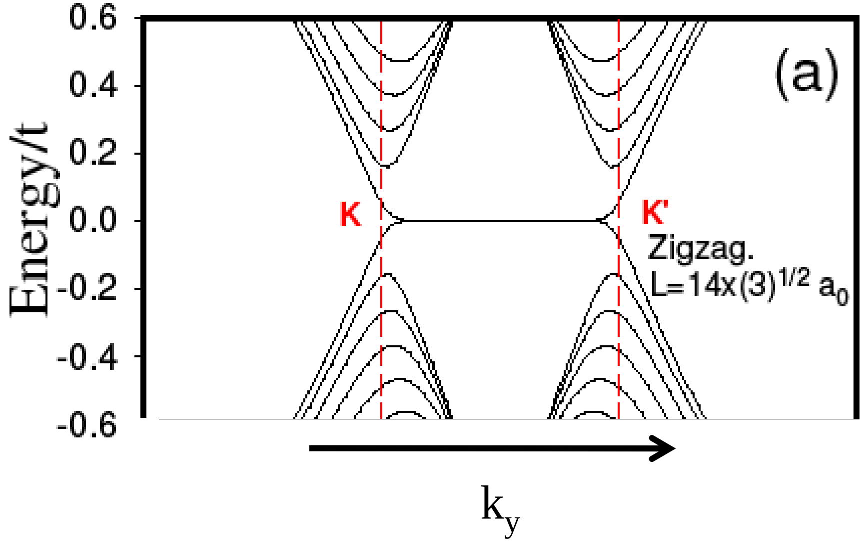
Basic component: Graphene ribbon

Two high symmetry directions for creating ribbon edges in graphene:



- Just nearest neighbor hopping
- Easily solve for states and spectrum in tight-binding.
- Results may be understood from Dirac equation.

Zigzag ribbon: tight-binding results



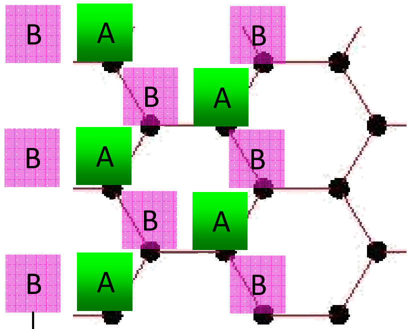
Lowest subband:

- Chiral edge mode
- Zero energy states, confined to edge
- "Valleytronics"

Continuum description: £+{ >| , @ £+{ ,h ln| |

s _ 6w / 5 d3 E E C lC{ ln| 3 lC{ . ln| 3 3 3 3 3 3 lC{ ln| 3 3 lC{ . ln| 3 F F D E E C D ≯N +{ , E ≯N +{ , F F D @ % E E C D ≯N 3+{ , E ≯N 3+{ , D ≯N +{ , E ≯N +{ , F F D D ≯N 3+{ , E ≯N 3+{ ,

What is the appropriate boundary condition?



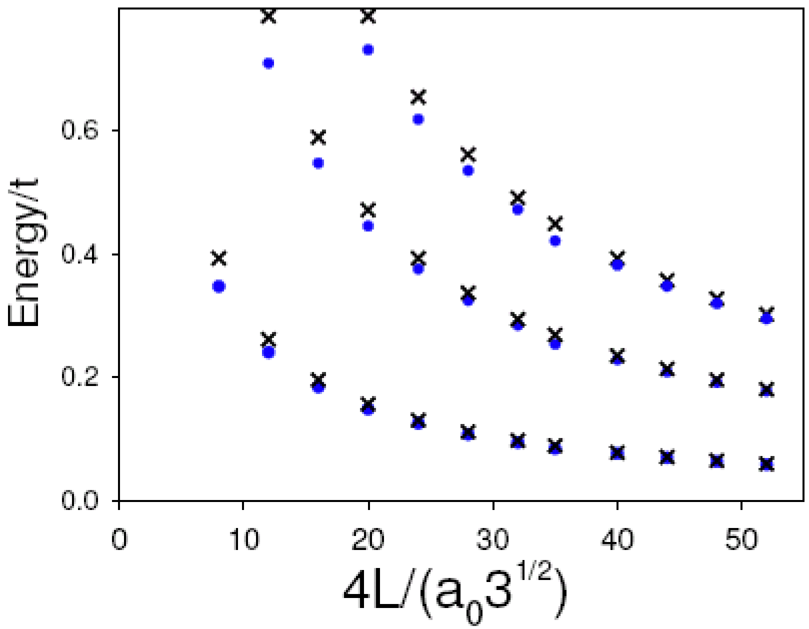
Boundary condition:
$\phi_{B,(K,K')}(x=0)=0$
for each valley separately.

Missing row of atoms all from same sublattice

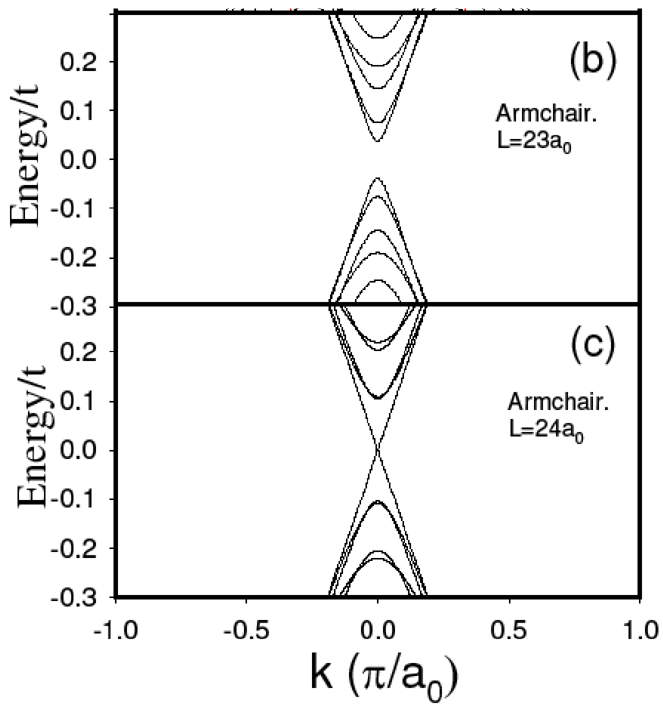
Resulting energies:

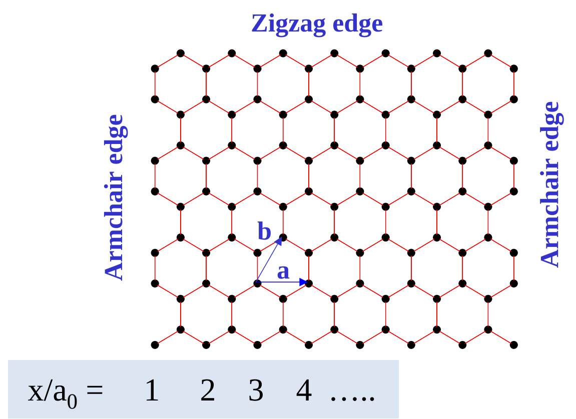
● = tight-binding

x = Dirac equation

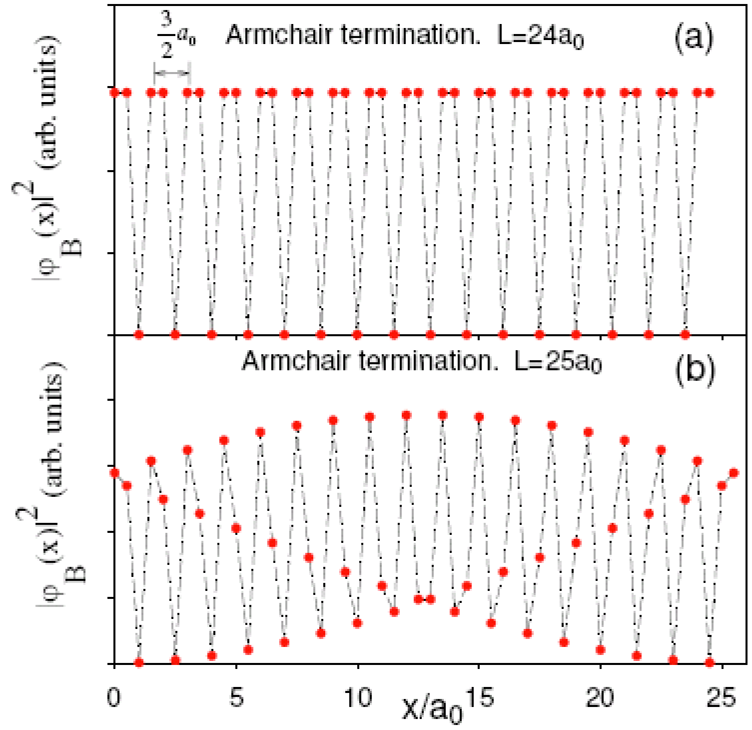


Armchair ribbon: tight-binding results

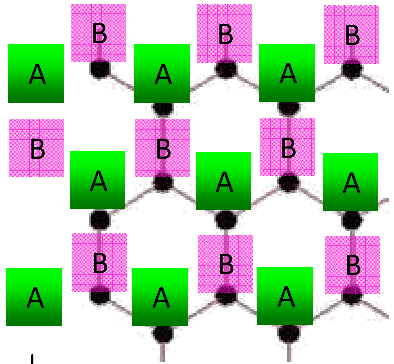




- Two of every three widths gapped
- Valleys overlap in this orientation
- Transverse wavefunctions have rapid oscillations



For armchair ribbons, boundary condition admixes valleys.



Boundary conditions:
$\phi_B(x=0)+\phi'_B(x=0)=0$
$\phi_A(x=0)+\phi'_A(x=0)=0$
Admixes valleys

Missing row of atoms with equal number of atoms from both sublattices

Boundary conditions for both edges fixes transverse wavevector:

$$\kappa_n = \frac{\pi}{W}\left(n + \frac{j}{3}\right)$$

j = 0,1, or 2 = remainder of (#columns)/3

$$\varepsilon_n = \pm\hbar v\sqrt{\kappa_n^2 + \kappa_y^2}$$

$\Longrightarrow$ j = 0 ribbons have gapless spectra and are metallic when undoped.

II. Graphene Junctions

Metallic (j=0) armchair ribbons are interesting and relatively simple to work with:

- Transverse wavefunctions do not depend on k_y
- 1D Dirac spectrum
- Interesting symmetry property:

$$n_q \geqslant n_| + \{ > | , @ \; s \frac{4}{50} \; '' \; \frac{4}{\frac{n_q \, . \, ln_|}{n}} \; N \; h^{ln_q \{} \; '' \; \frac{4}{\frac{n_q \, . \, ln_|}{n}} \; N^3 \; h^{¥ \, ln_q \{} \; h^{ln_| \, |} >$$

Can show

$$D \geqslant N \; ' \; l \; E \geqslant N^3$$
$$E \geqslant N \; ' \; l \; D \geqslant N^3$$

yields a w/f at same energy which satisfies appropriate boundary condition.

Express in terms of a matrix:

$$T = \begin{bmatrix} 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}$$

$$\hat{T};H] = 0; \quad T^2 = 1; \quad \text{Eigenvalues of } T = 1$$

- Matrix maps state with $k_n > 0$ to state with $k_n < 0$.
- States with $k_n = 0$ are special:

$$_{0,p_y}(x,y) = p\frac{1}{2W} \binom{1}{i\,\mathrm{sgn}(k_y)}_K \binom{1}{i\,\mathrm{sgn}(k_y)}_{K'} e^{ik_y y}$$

$$\Longrightarrow \quad T\,_{0,k_y} = \mathrm{sgn}(\%)\,\mathrm{sgn}(k_y)\,_{0,k_y}$$

Lowest subband states of metallic AC ribbons are *chiral*.

So what happens at a junction? Can the chirality be preserved?

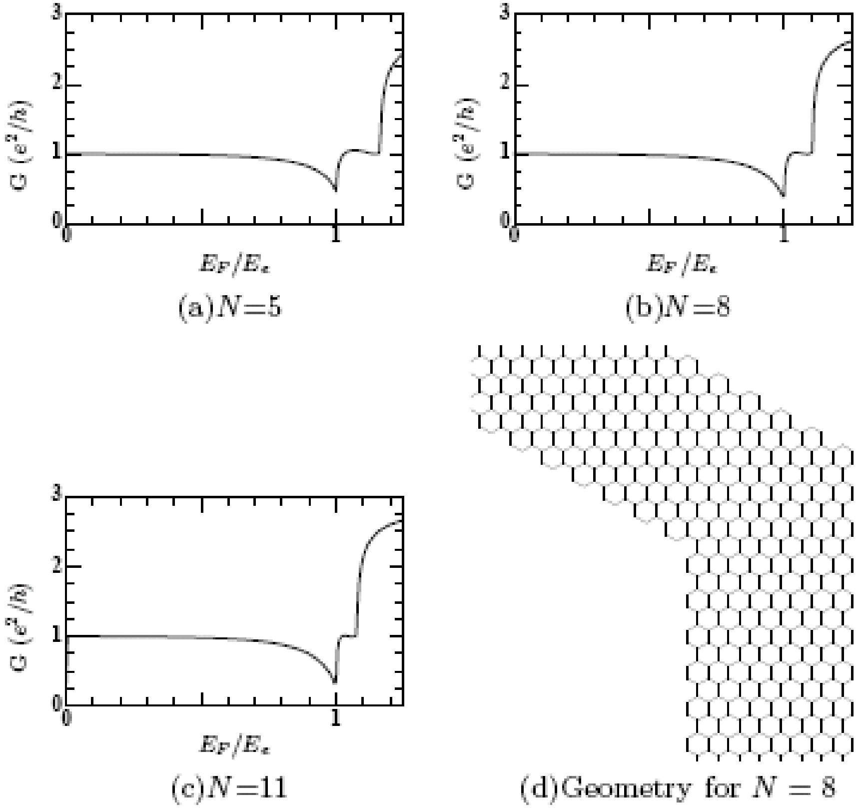
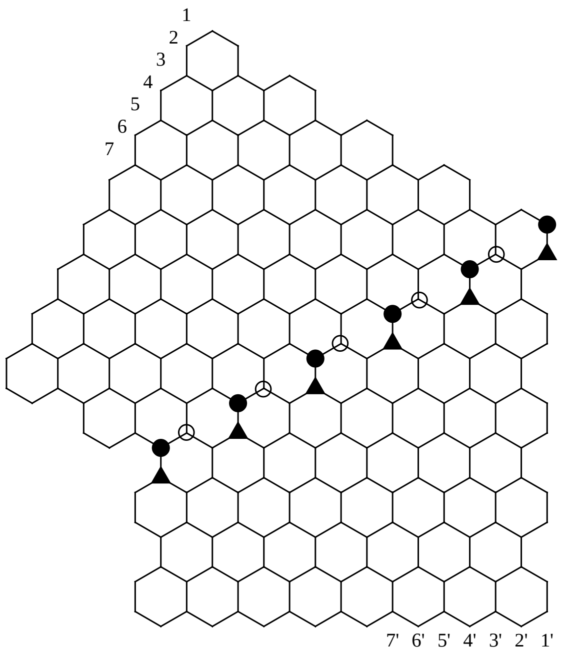


FIG. 4: Conductance per spin of 120-degree bends in armchair nanoribbons having N transverse channels. Geometry for N=8 illustrated in (d).

Yes, for appropriately formed junction.

Result may be understood via *single mode approximation*.



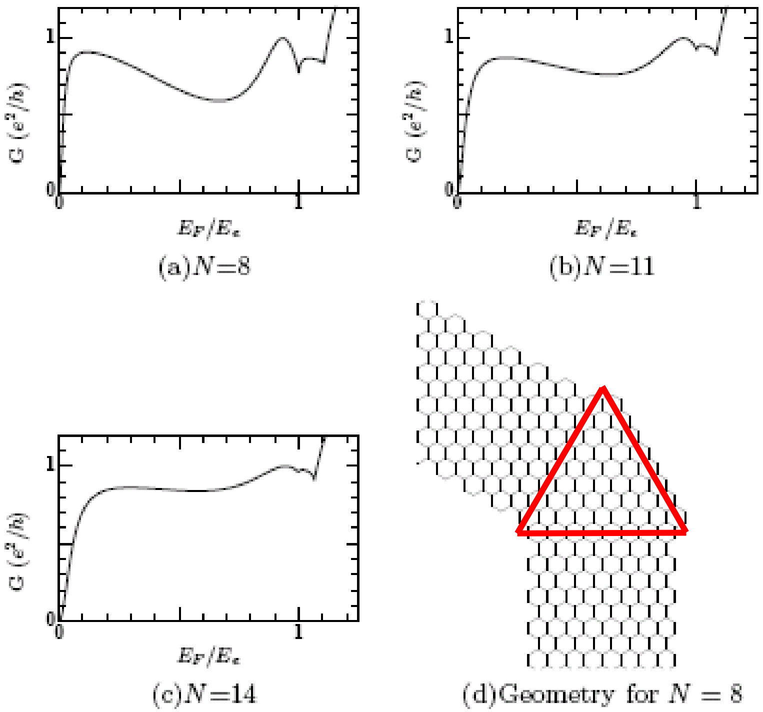
• Match ribbon wavefunctions (○, ●) and current (▲) along joining surface.

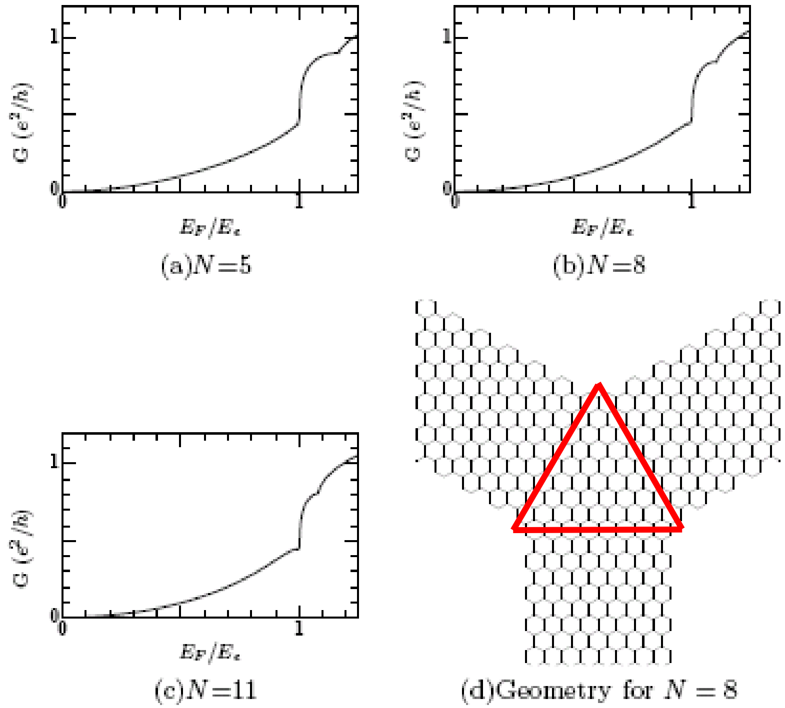
• Transmission amplitude proportional to overlap on joining surfaces:

P 3>3 +s| , , ∪ g +4, 3>s| +{+ ,>|+ ,, +5,¤ 3>s| +{+ ,>|+ ,,

For $p_y \longrightarrow 0$, find $M_{0,0} = \pm i$!

Other kinds of junctions give more complicated results.

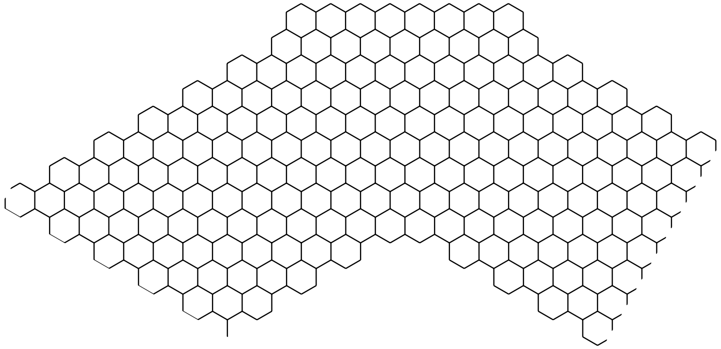




Transmission through equilateral triangles.

Single mode approximation….

1. Two-lead triangle.



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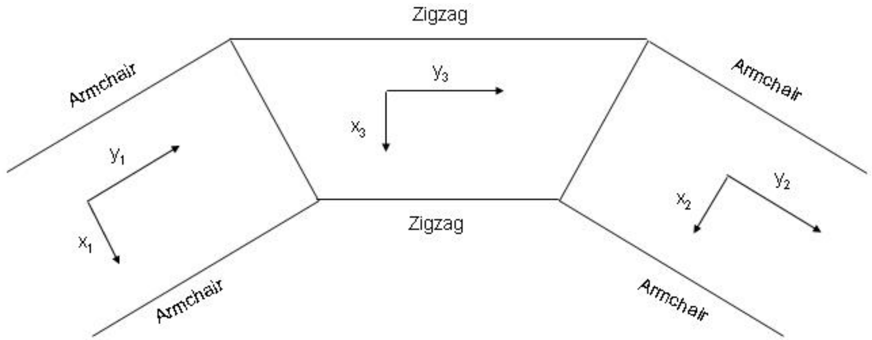
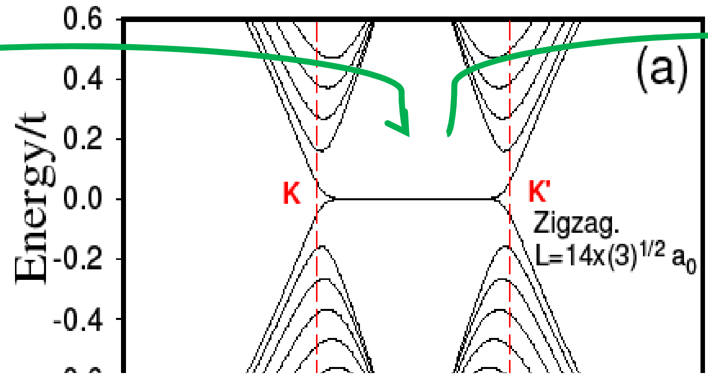


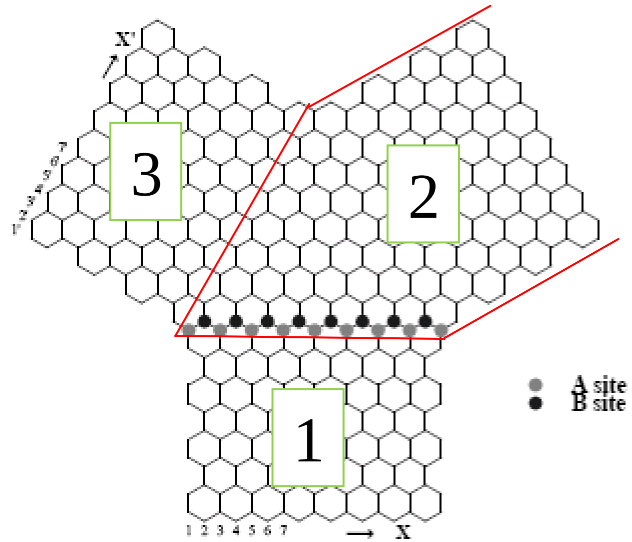
Confined state



Confined state

⇒ Suppressed transmission at low energy

2. Three-lead triangle: view as two-step transmission.



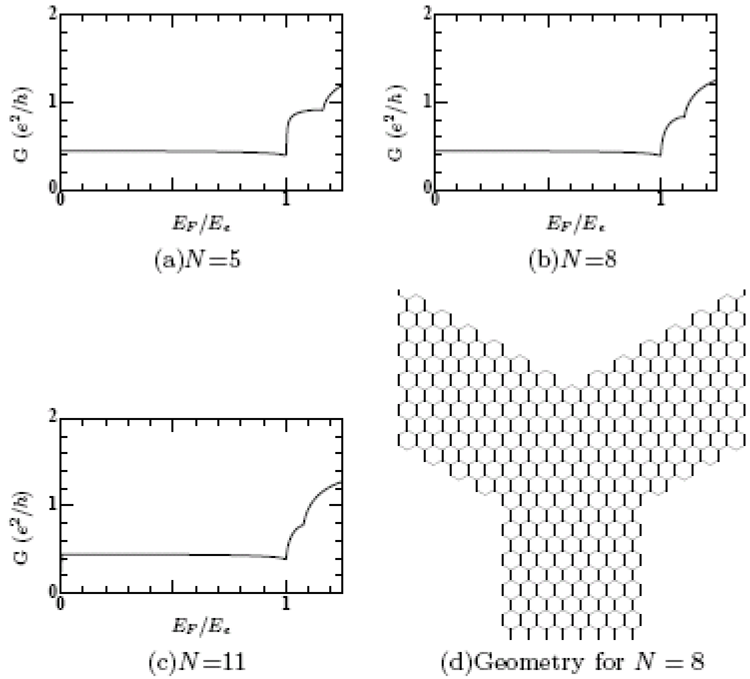
Find in limit $p_y \longrightarrow 0$, overlap between lowest subbands of

1 and 2

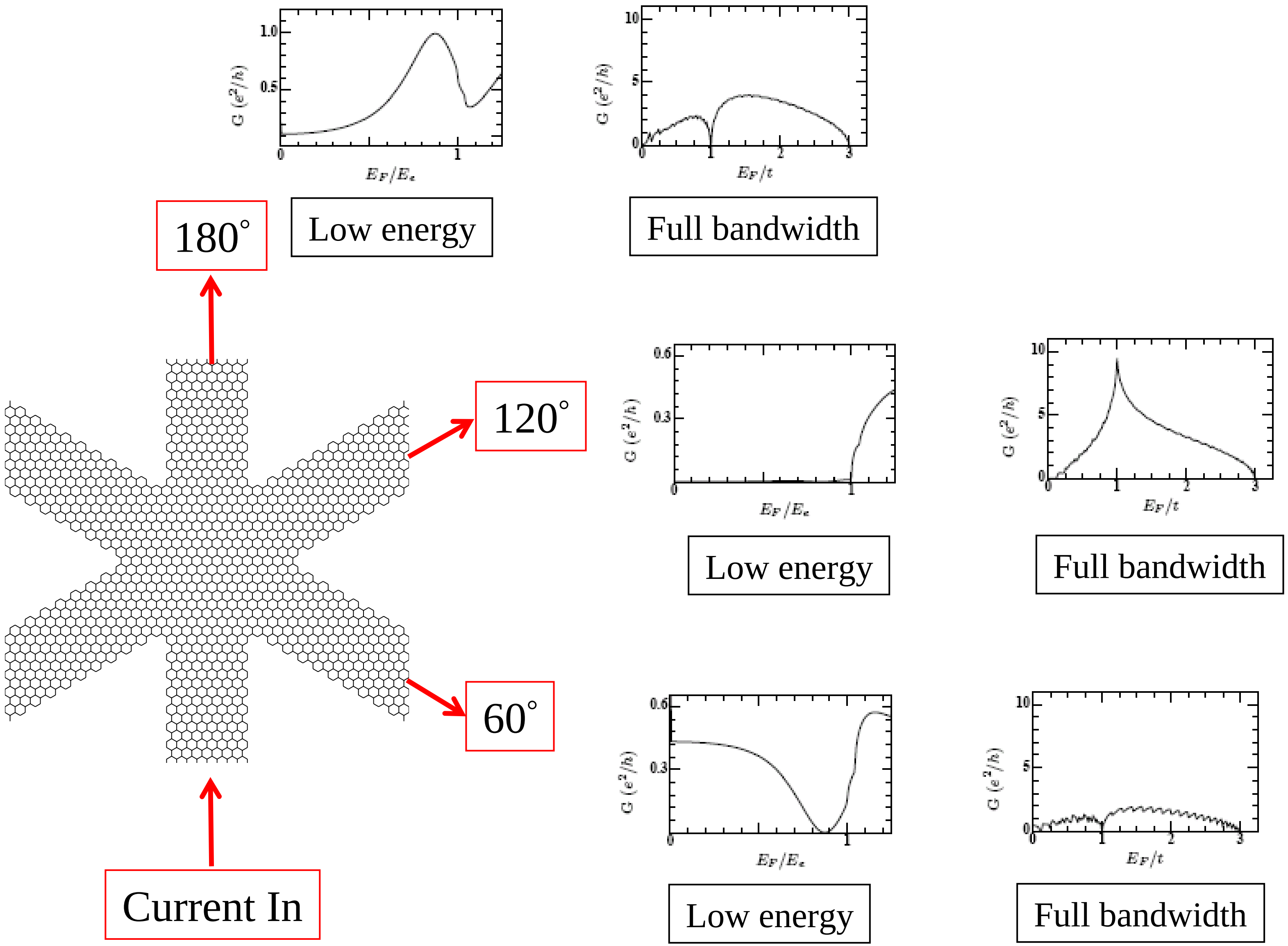
vanish on joining surface.

$\Rightarrow$ Vanishing transmission in SMA

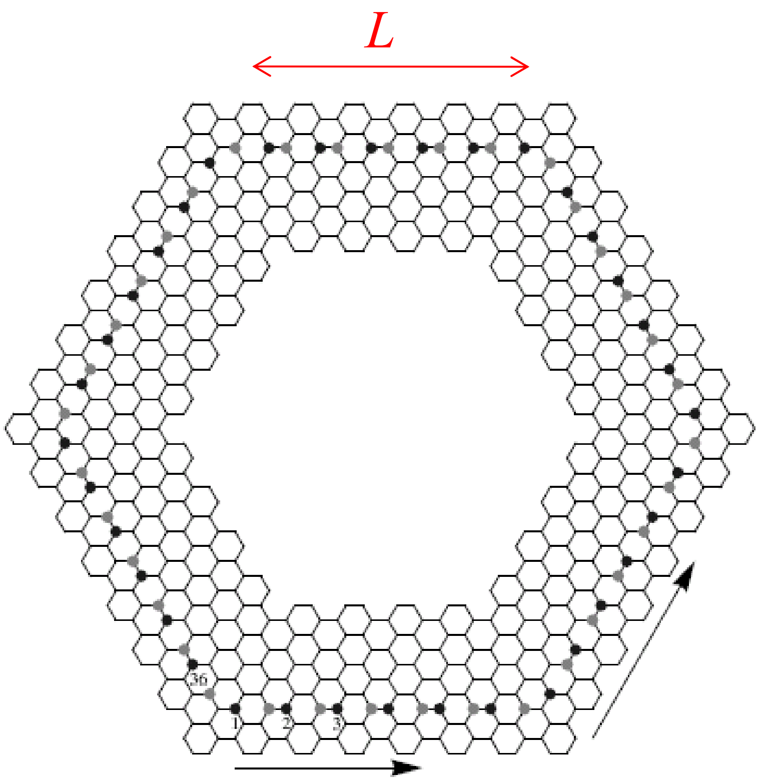
Note importance of corner geometry:

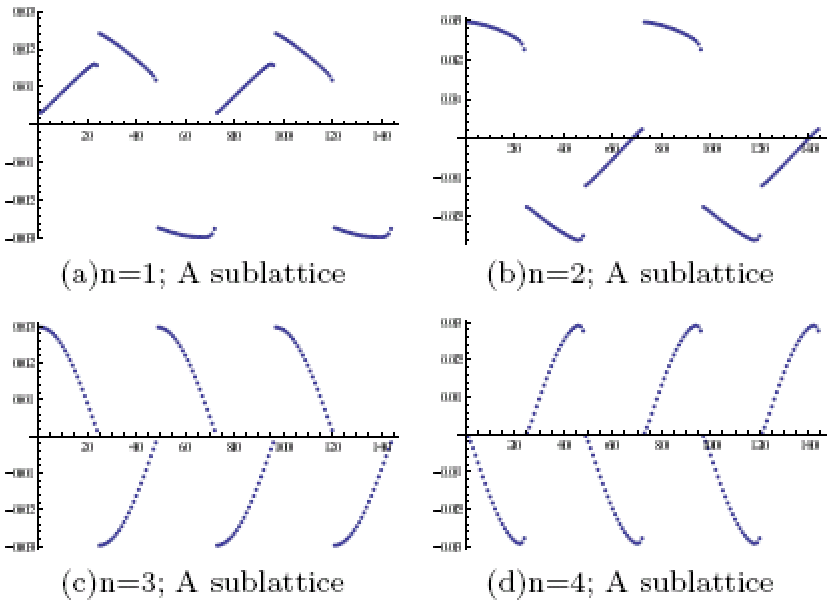


Transmission through hexagons:



III. Armchair Rings: Breaking Effective Time Reversal Symmetry





(a)n=1; A sublattice

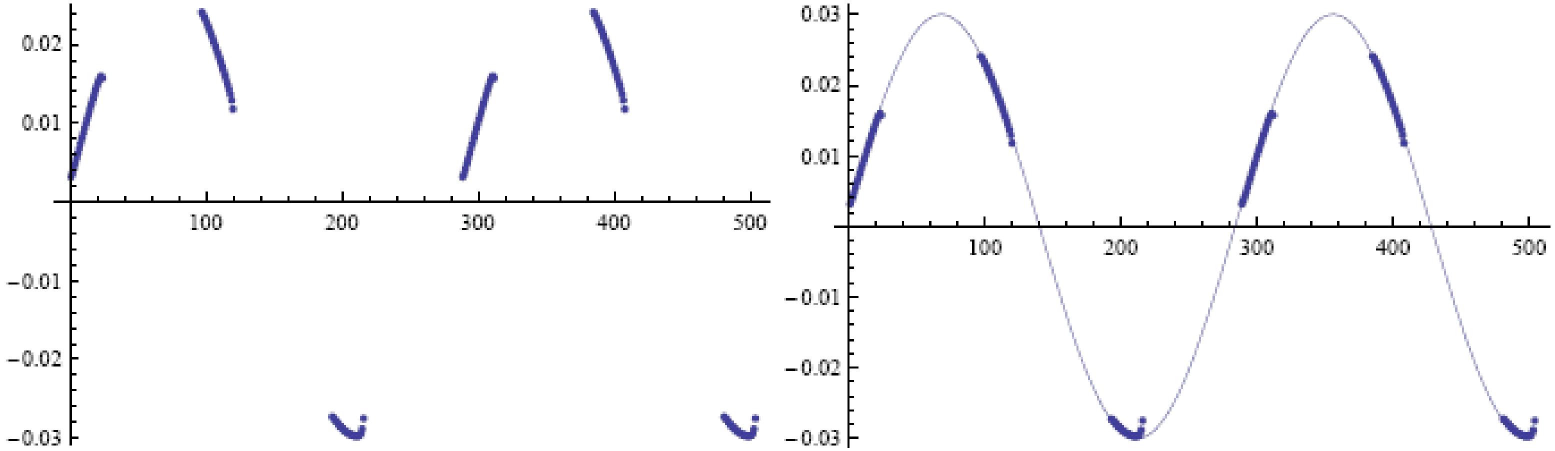
(b)n=2; A sublattice

(c)n=3; A sublattice

(d)n=4; A sublattice

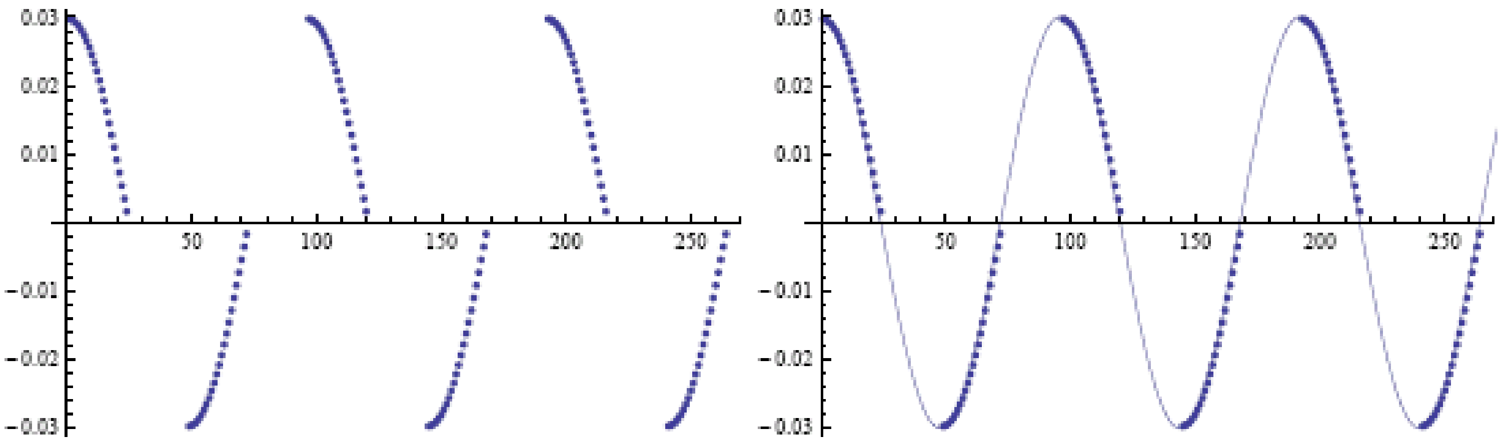
Wavefunctions have discontinuities at corners.

+|,2 vlq^S|| . 3+|,



(a) $P_y L = \pi/6$, insert $\pi/2$ between each arm

(b) Fit it with a *sin* function



(a) $P_y L = \pi/2$, insert $\pi/2$ between each arm

(b) Fit it with a *sin* function

Summary of fits for lowest energy levels:

Measured from E=0

Rotational quantum number

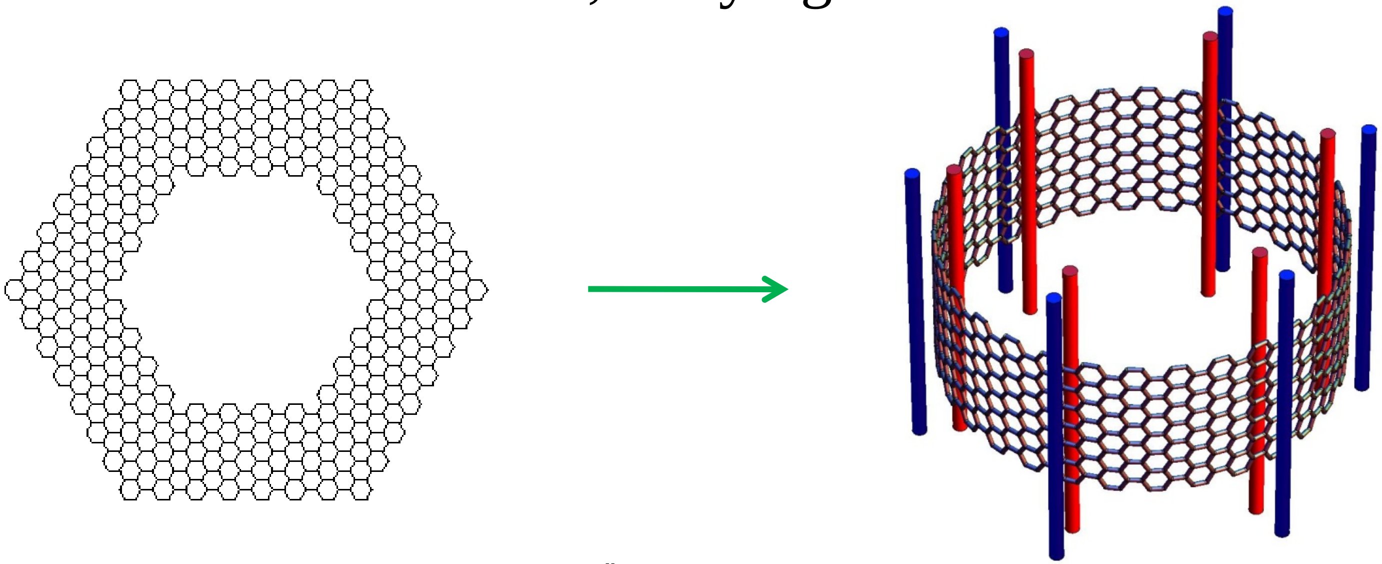
Energy level	$P_y L$	θ_0	n
1	$\pi/6$	$\pi/2$	2
2	$-\pi/6$	$-\pi/2$	-2
3	$\pi/2$	$\pi/2$	3
4	$-\pi/2$	$-\pi/2$	-3
5	$5\pi/6$	$\pi/2$	4
6	$-5\pi/6$	$-\pi/2$	-4

Notice: h[1]″3 @ lvjq+S| ,vjq+%,

Levels satisfy: 9 +S|O . 3,@ 5 p

⇒ Continuity of wavefunctions around ring, when phase jumps included.

At low energy, ring with 60° corners is equivalent to annulus with "flux" tubes, carrying



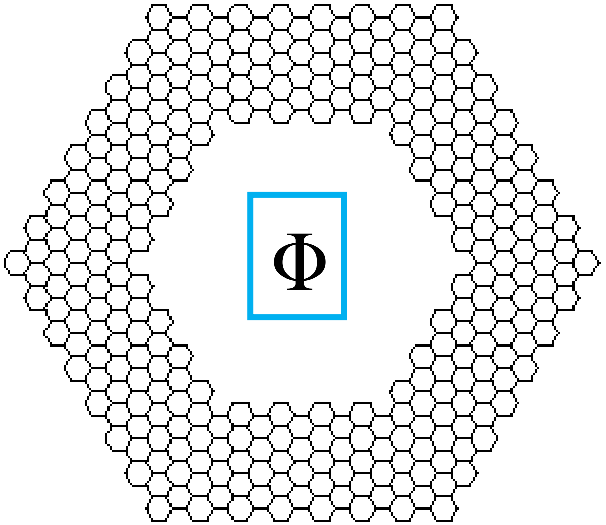
$ h1¨ 3 @ —W +|,
5

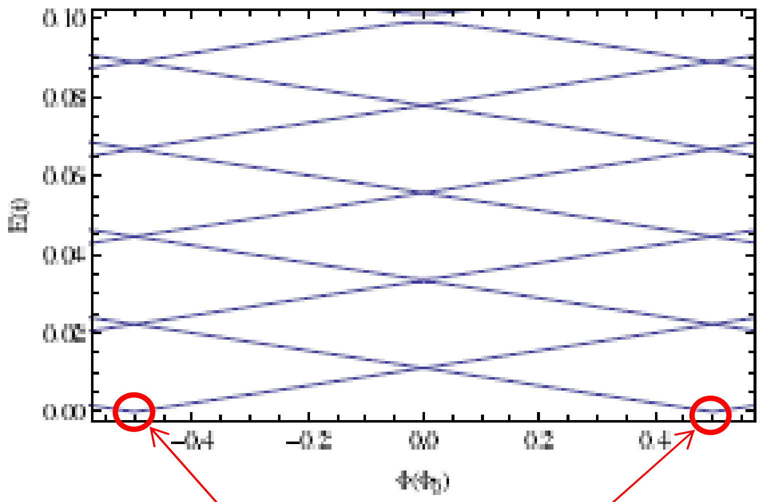
K +s , sq >s| @ % sq >s| $ K +s D , 3 sq >s| @ % 3 sq >s|

D +|, @ g/g| a

- ψ' everywhere continuous
- "Broken effective time-reversal symmetry"
- Analog of gauge fields from disclinations:
  Vozmediano et al, 1993

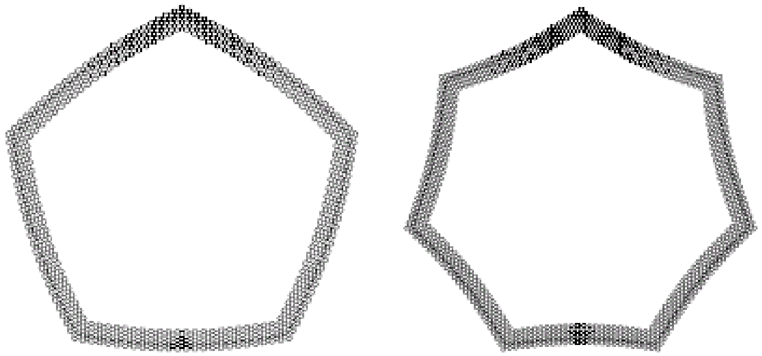
Because net effective flux through ring is different than zero for each eigenvalue of T, P_y=0 ($\varepsilon = 0$) not an allowed eigenvalue. But effective flux may be cancelled by real magnetic flux.



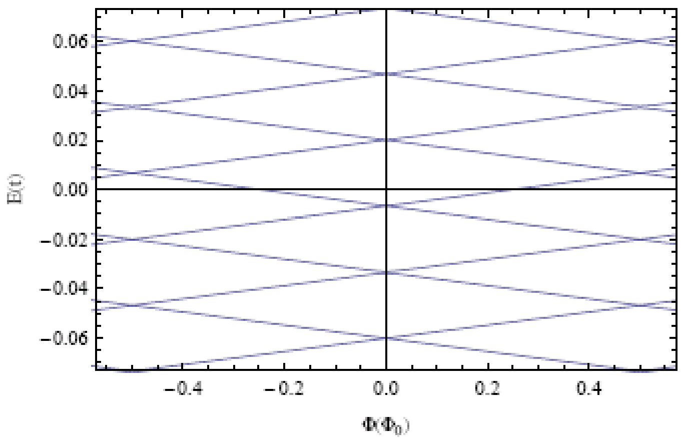


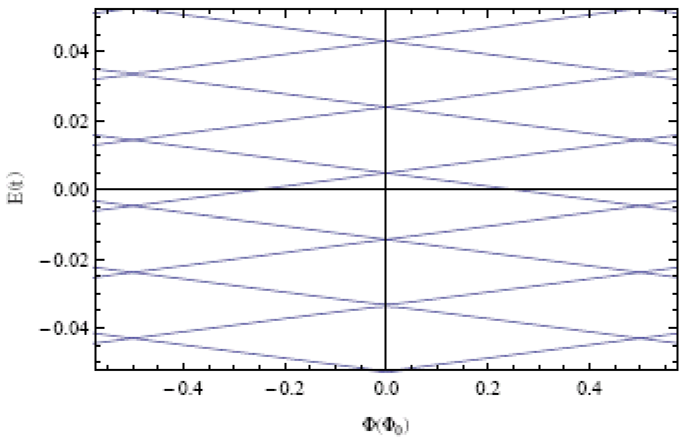
Effective flux cancelled when half flux quantum applied through ring

Pentagons and Heptagons



- When bonds undistorted these live on surface with curvature
- Effective flux through ring is $\pm(5/4)\Phi_0$, $\pm(7/4)\Phi_0$.





- Particle-hole symmetry broken: a topological property of network
- P_y=0 state restored at quarter flux
- Signature of broken effective time-reversal symmetry

IV. Graphene in a Superlattice Potential

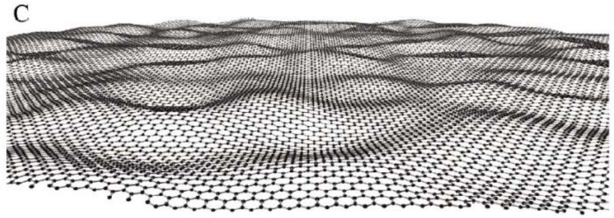
Ripples in graphene: possibility of periodic modulations?

nature Vol 446|1 March 2007|doi:10.1038/nature05545

LETTERS

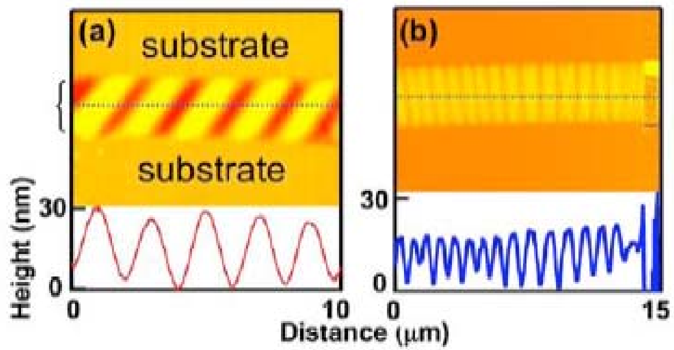
The structure of suspended graphene sheets

Jannik C. Meyer[1], A. K. Geim[2], M. I. Katsnelson[3], K. S. Novoselov[2], T. J. Booth[2] & S. Roth[1]



Ripple Texturing of Suspended Graphene Atomic Membranes

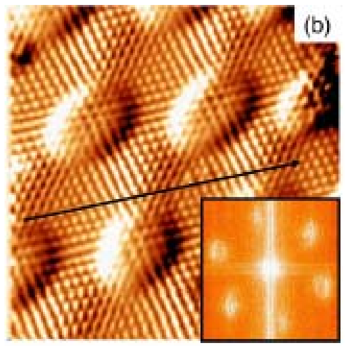
Wenzhong Bao[1], Feng Miao[1], Zhen Chen[2], Hang Zhang[1], Wanyoung Jang[2], Chris Dames[2], Chun Ning Lau[1*]



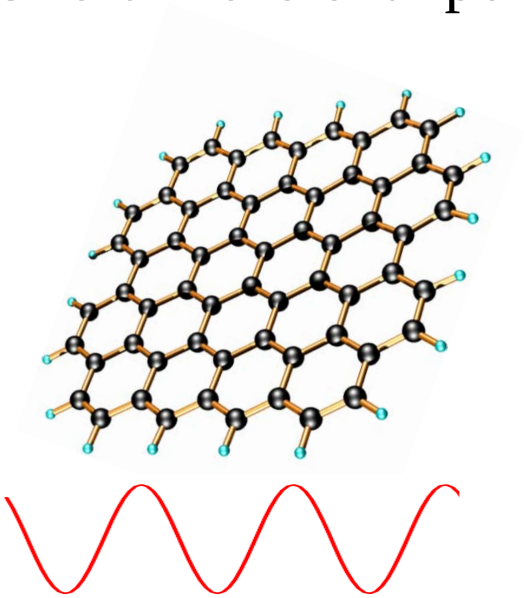
PRL 100, 056807 (2008) PHYSICAL REVIEW LETTERS week ending 8 FEBRUARY 2008

Periodically Rippled Graphene: Growth and Spatially Resolved Electronic Structure

A. L. Vázquez de Parga,[1] F. Calleja,[1] B. Borca,[1] M. C. G. Passeggi, Jr.,[2] J. J. Hinarejos,[1] F. Guinea,[3] and R. Miranda[1,4]



One-dimensional periodic potential:



$$V(x) = V_0 \cos G_0 x$$

$$\begin{cases} \dfrac{2\pi}{G_0} >> a \\ V_0 << t \end{cases}$$

Dirac equation for a single valley and spin,

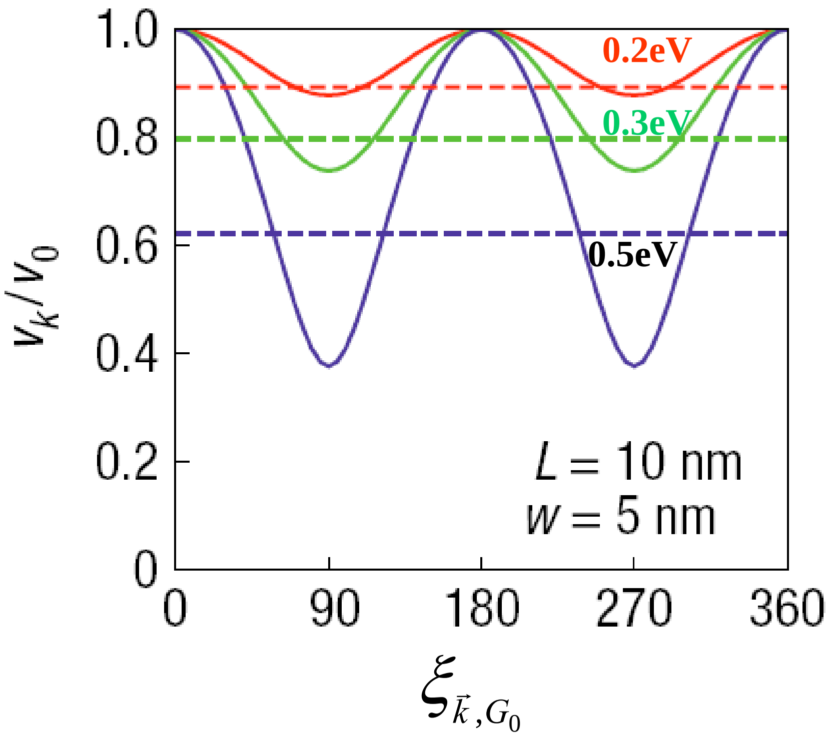
$$H = \hbar v_F \left(-i\sigma_x \partial_x - i\sigma_y \partial_y \right) + V(x) I = \begin{pmatrix} V(x) & -i\partial_x - ik_y \\ -i\partial_x + ik_y & V(x) \end{pmatrix}$$

$\sigma_{x,y}$, Pauli matrices
I: identity
$[H,\partial_y]=0 \Rightarrow k_y$ is a good quantum number, $e^{ik_y y}$
Wave function has 2 components (2 sublattices that make up the honeycomb lattice).

nature physics | VOL 4 | MARCH 2008 | www.nature.com/naturephysics

Anisotropic behaviours of massless Dirac fermions in graphene under periodic potentials

CHEOL-HWAN PARK[1,2], LI YANG[1,2], YOUNG-WOO SON[3], MARVIN L. COHEN[1,2] AND STEVEN G. LOUIE[1,2*]



$$\frac{v_{\vec{k}} - v_0}{v_0} = -\frac{V_0^2}{\hbar^2 v_F^2 G_0^2} \sin^2 \xi_{\vec{k},G_0}$$

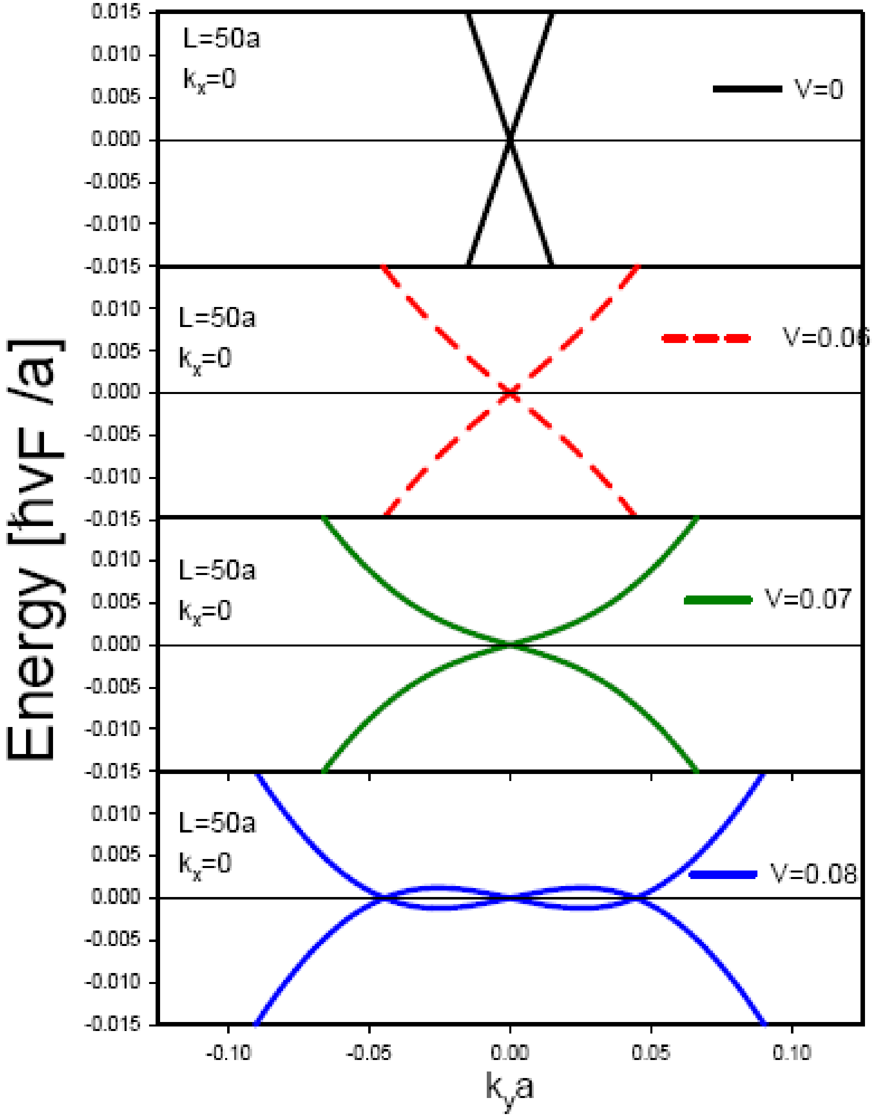
Electron Beam Supercollimation in Graphene Superlattices

Cheol-Hwan Park,[†,‡] Young-Woo Son,[§,‖] Li Yang,[†,‡] Marvin L. Cohen,[†,‡] and Steven G. Louie[*,†,‡]

NANO LETTERS
2008
Vol. 8, No. 9
2920-2924

What happens if we continue to increase V_0? Does the velocity go to zero?
What signature can be seen in transport?

Emerging zeros energy states:



Band structure obtained
by diagonalizing the Hamiltonian
expanded in plane waves.

Unitary transformation $H' = U_1^+ H U_1$

(Park et al. , 2008)

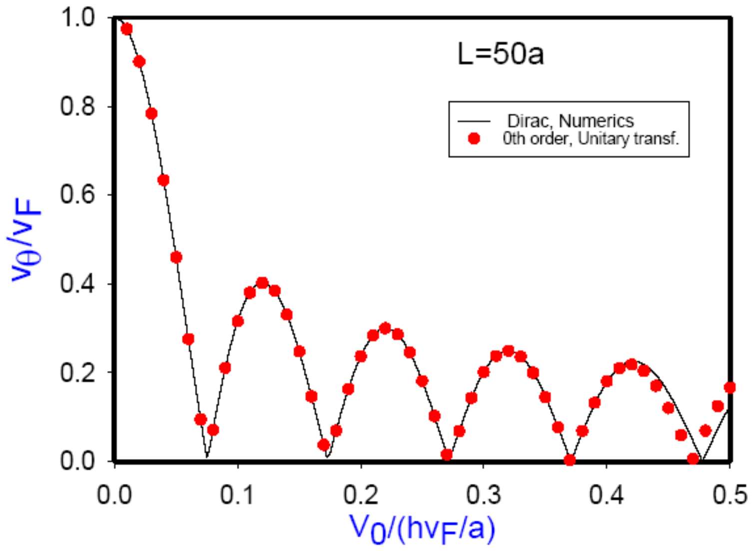
$$U_1 = \begin{pmatrix} e^{-i\frac{\alpha(x)}{2}} & -e^{i\frac{\alpha(x)}{2}} \\ e^{-i\frac{\alpha(x)}{2}} & e^{i\frac{\alpha(x)}{2}} \end{pmatrix}$$

with $\alpha(x) = \frac{2}{\hbar v_F} \int_0^x V(x')dx'$

$$H' = \hbar v_F \begin{pmatrix} -i\partial_x & -ik_y e^{i\alpha(x)} \\ ik_y e^{-i\alpha(x)} & i\partial_x \end{pmatrix}$$

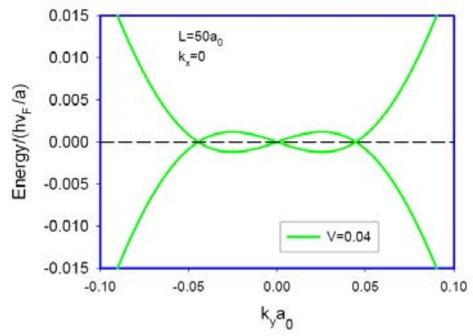
$$e^{i\alpha(x)} = J_0\left(\frac{2V_0}{\hbar v_F G_0}\right) + \sum_{l \neq 0} J_l\left(\frac{2V_0}{\hbar v_F G_0}\right) e^{ilG_0 x}$$

$$\varepsilon(\vec{k}) = \hbar v_F \sqrt{k_x^2 + k_y^2 J_0^2\left(\frac{2V_0}{\hbar v_F G_0}\right)}$$



- Pert theory explains group velocity near original Dirac point
- Results depend on V_0/G_0
- Does not explain emergent zero modes

Searching for zero modes (1)



$$\begin{pmatrix} -i\partial_x & -ik_y e^{i\alpha(x)} \\ ik_y e^{-i\alpha(x)} & i\partial_x \end{pmatrix} \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix} = 0$$

$$\phi_A = \phi_B^* = \phi$$

$$\partial_x \phi + k_y e^{i\alpha} \phi^* = 0$$

$$\phi = |\phi| e^{i\chi}$$

$$\begin{cases} k_y \sin(\alpha - 2\chi) + \partial_x \chi = 0 \\ |\phi| \propto \exp\left\{ -k_y \int_{x_0}^{x} \cos[\alpha(x') - 2\chi(x')] dx' \right\} \end{cases}$$

Boundary conditions: Bloch state, $\phi(x + L_0) = e^{ik_x L_0} \phi(x)$

$$i)\ \ \chi(x + L_0) = \chi(x) + 2\pi \,\mathrm{m}$$

$$ii)\ \int_0^{L_0} \cos[\alpha(x) - 2\chi(x)] dx = 0$$

Mechanical analog

$$k_y \sin(\alpha - 2\chi) + \partial_x \chi = 0$$

Writing $\bar{\chi} = 2\chi - \alpha, \quad x \to t$

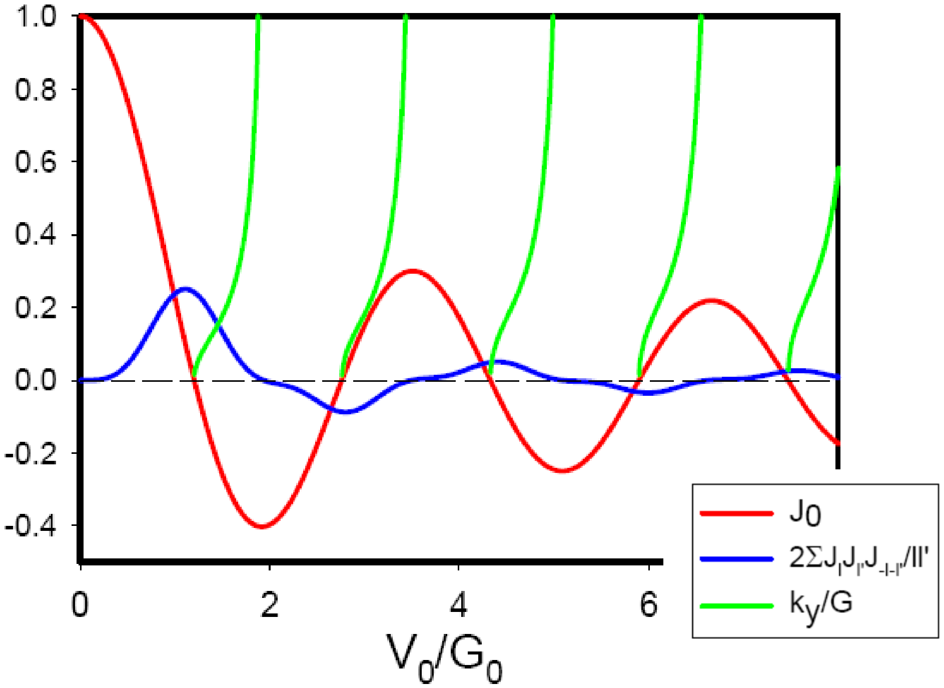
$$-\partial_t \bar{\chi} - \partial_t \alpha + 2k_y \sin \bar{\chi} = 0$$

Eq. of motion for position $\bar{\chi}$ of an overdamped particle, subject to a periodic time dependent potential $\partial_t \alpha$ and a spatially periodic force $2k_y \sin\bar{\chi}$.

Generic solution is not periodic. However for certain parameters periodic solutions can be found.

Solve perturbatively in k_y: $\chi = k_y \chi^{(1)} + k_y^2 \chi^{(2)} + \ldots$

Find: $$\left(\frac{k_y}{G_0}\right)^2 = -\frac{J_0\left(2V_0/\hbar v_F G_0\right)}{2\sum_{l_1,l_2\,\mathrm{odd}} J_{l_1} J_{l_2} J_{-l_1-l_2}/l_1 l_2}$$

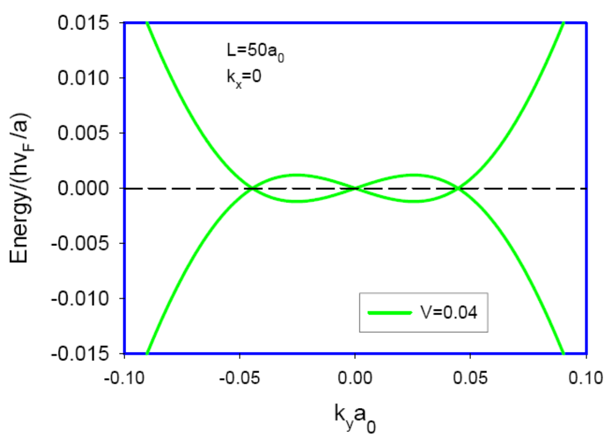


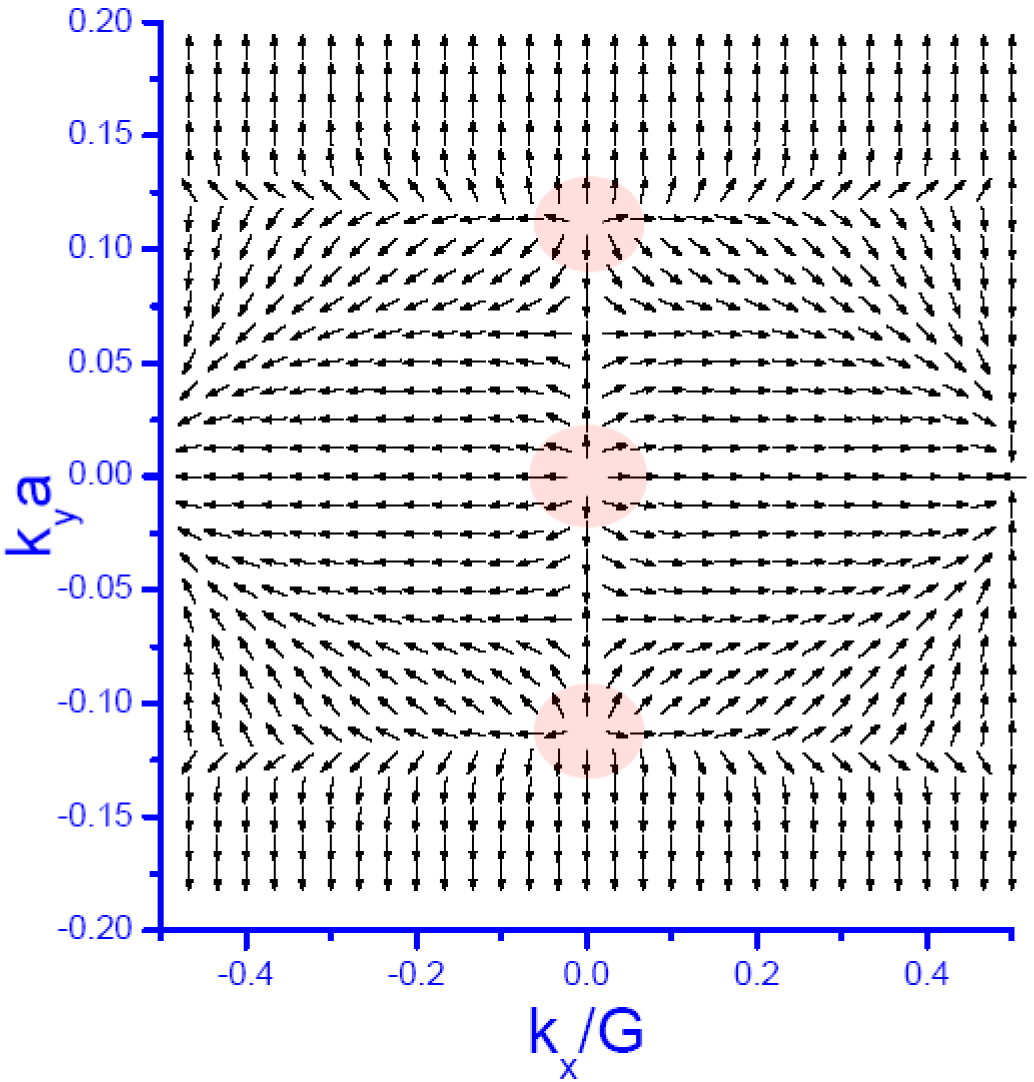
Get a new zero mode every time J_0 passes through zero!

Zero modes are Dirac points

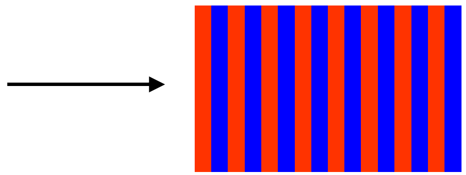
$$<\sigma_x(\vec{k})>, <\sigma_y(\vec{k})>$$

Evaluated in the lowest positive energy band.





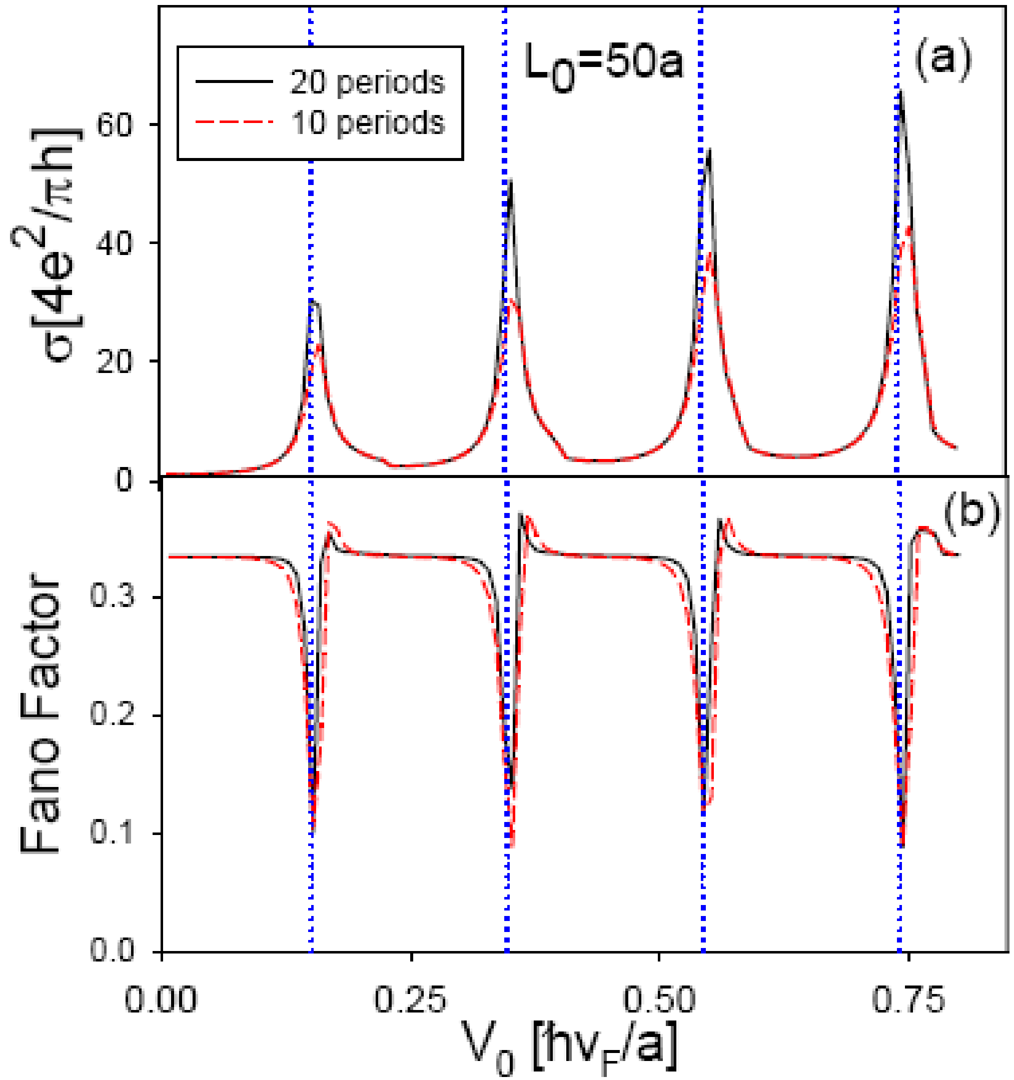
Conductivity



$$G = \frac{4e^2}{h}\sum T_n , \quad F = \frac{\sum T_n(1-T_n)}{\sum T_n}$$

$$\sigma = \frac{L}{W} G$$

Also: In magnetic field,
new Dirac points lead to
enhanced Hall conductivity
(Park et al., ArXive:0903.3091)



V. Summary

- Mesoscopic transport in graphene support diverse phenomena
- Graphene armchair ribbons: chiral transport in lowest subband when metallic
- Junctions may be perfect transmitters but introduce phase jumps which act like effective flux wrapped around ribbon
- Different possible interference effects in transport through polygons
- Graphene rings have spectra which reflect "effective time-reversal symmetry breaking"
- Two-dimensional graphene in periodic potential support
  - anisotropic Dirac point
  - emerging Dirac points at large V_0/G_0
  - signatures in transport of their emergence

Refs: A.P. Iyengar, T. Luo, HAF, L. Brey PRB **78**, 235411 (2008)

L. Brey and HAF, PRL (to appear – ArXive:0904.0540)

T. Luo, A.P. Iyengar, HAF, L. Brey (ArXive:0907.3150)