Domain Walls in Gapped Graphene

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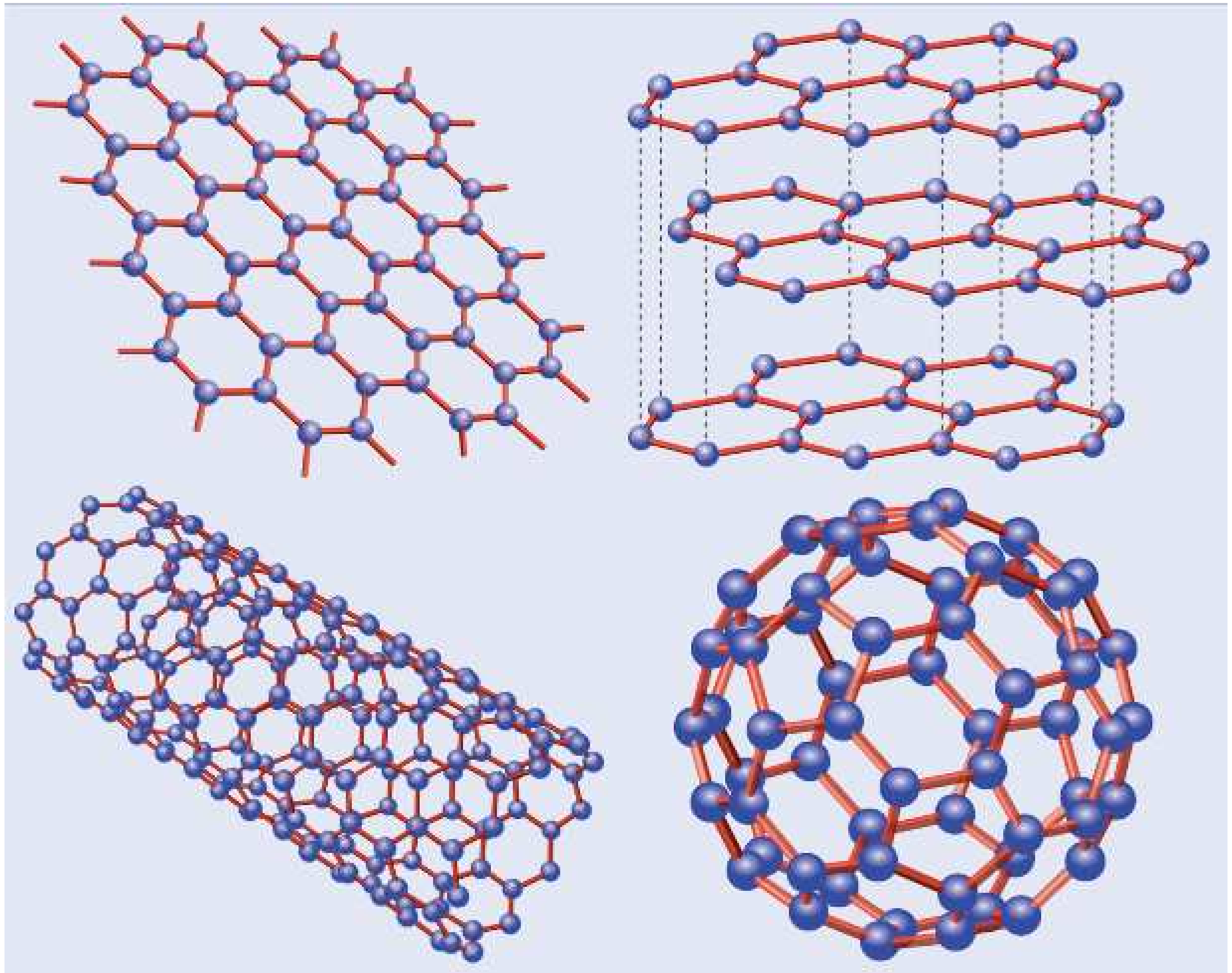
University of British Columbia

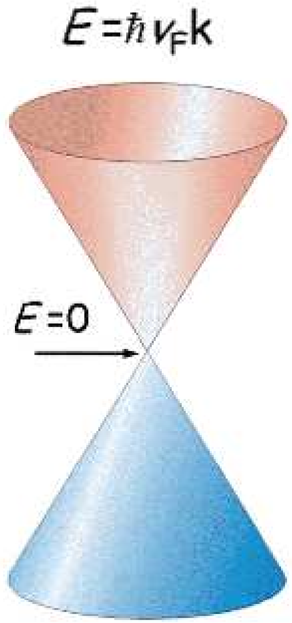
Exact results in two dimensional field theory, GGI, September 2008

Graphene is a 2-dimensional array of carbon atoms

with a hexagonal lattice structure



Electron spectrum



Band structure and linear dispersion relation $E(\vec{k}) = \hbar v_F |k|$

P. R. Wallace, *Phys. Rev. 71, 622 (1947)*

J. C. Slonczewsi and P. R. Weiss, *Phys. Rev. 109, 272 (1958).*

Dirac equation

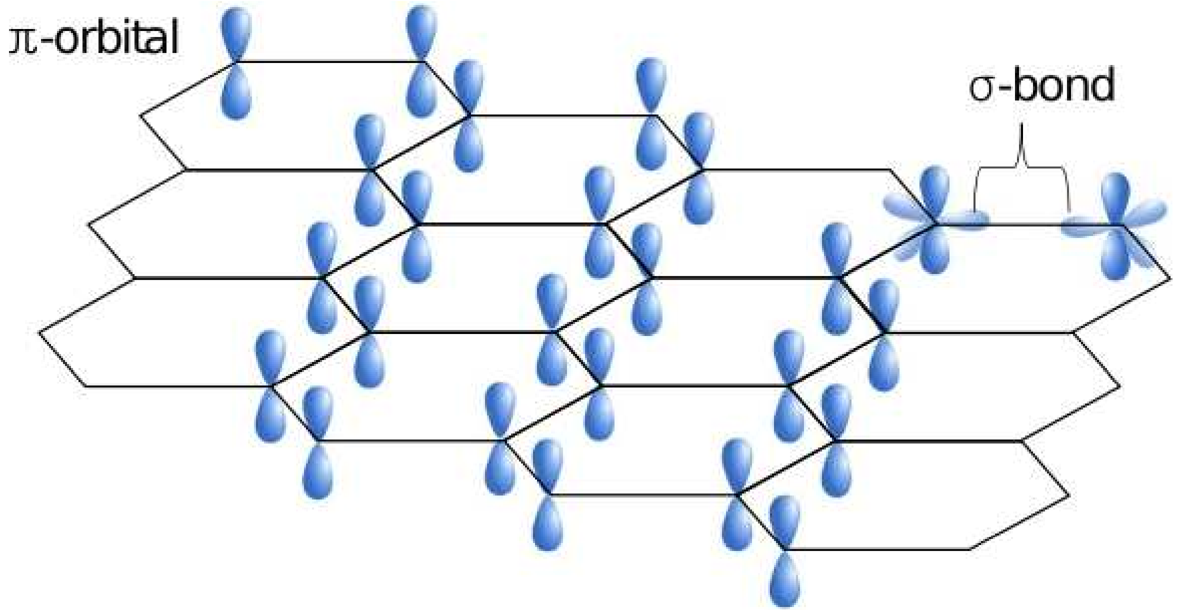
G. W. S., *Phys. Rev. Lett. 53, 2449 (1984)*

For many years **Graphene** was a *hypothetical* material

Graphene was produced and identified in the laboratory in 2004

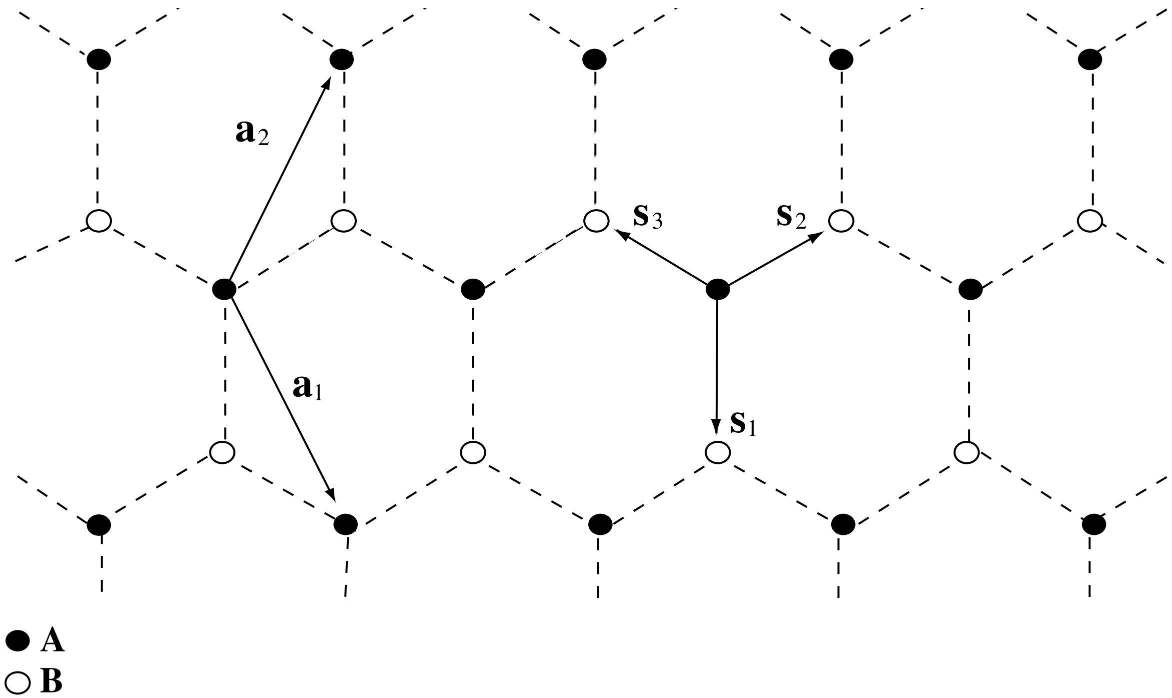
- Micromechanical cleavage of bulk graphite up to 100 micrometer in size via adhesive tapes !

Novoselov et al, Science **306**, 666 (2004)



A carbon atom has four valence electrons. Three of these electrons form strong covalent σ-bonds with neighboring atoms. The fourth, π-orbital is un-paired.

Tight-binding model



hexagonal lattice = two triangular sub-lattices $\vec{A}$ and $\vec{B}$ connected by vectors $\vec{s}_1, \vec{s}_2, \vec{s}_3$.

$$H = \sum_{\vec{A},i} \left(t \; b^{\dagger}_{\vec{A}+\vec{s}_i} a_{\vec{A}} + t^* \; a^{\dagger}_{\vec{A}} b_{\vec{A}+\vec{s}_i} \right)$$

Tight-binding model

$$H = \sum_{\vec{A},i} \left(t\ b^\dagger_{\vec{A}+\vec{s}_i} a_{\vec{A}} + t^*\ a^\dagger_{\vec{A}} b_{\vec{A}+\vec{s}_i} \right)$$

$$i\hbar \frac{da_{\vec{A}}}{dt} = t \sum_i b_{\vec{A}+\vec{s}_i} \quad , \quad i\hbar \frac{db_{\vec{B}}}{dt} = t^* \sum_i a_{\vec{B}-\vec{s}_i}$$

$$a_{\vec{A}} = e^{i\frac{E}{\hbar}t + i\vec{k}\cdot\vec{A}} a_0 \quad , \quad b_{\vec{B}} = e^{-i\frac{E}{\hbar}t + i\vec{k}\cdot\vec{B}} b_0$$

$$E \begin{bmatrix} a_0 \\ b_0 \end{bmatrix} = \begin{bmatrix} 0 & t\sum_i e^{i\vec{k}\cdot\vec{s}_i} \\ t^* \sum_i e^{-i\vec{k}\cdot\vec{s}_i} & 0 \end{bmatrix} \begin{bmatrix} a_0 \\ b_0 \end{bmatrix}$$

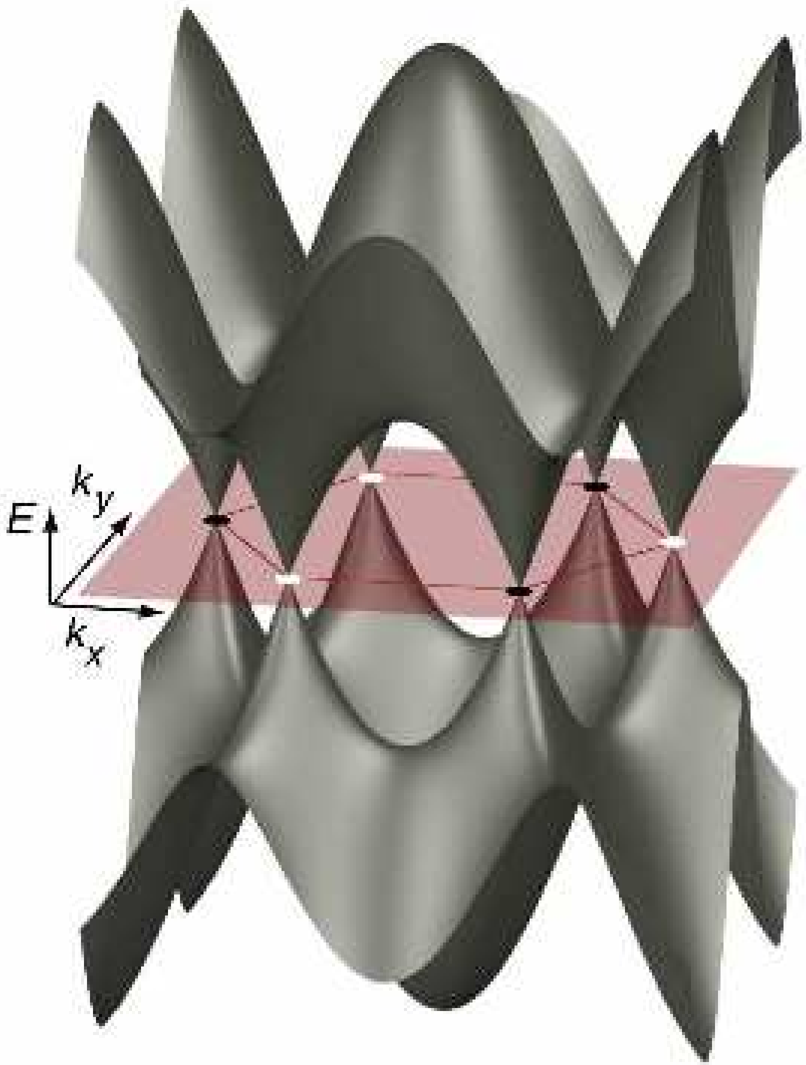
π-bands $E(k) = \pm|t|\sqrt{(1 + 2\cos(\frac{3k_y}{2})\cos(\frac{\sqrt{3}k_x}{2}))^2 + \sin^2(\frac{3k_y}{2})}$

Degeneracy points

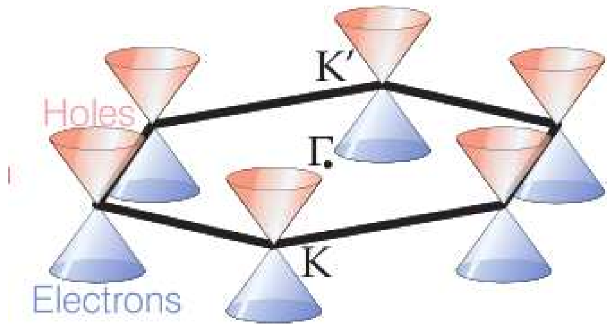
$$\sin(\frac{\sqrt{3}k_y}{2}) = 0 \rightarrow \cos(\frac{\sqrt{3}k_y}{2}) = 1 \ , \ \cos(\frac{3k_x}{2}) = -\frac{1}{2}$$

$$\sin(\frac{\sqrt{3}k_y}{2}) = 0 \rightarrow \cos(\frac{\sqrt{3}k_y}{2}) = -1 \ , \ \cos(\frac{3k_x}{2}) = \frac{1}{2}$$

Band structure of graphene



Linearize spectrum near degeneracy points



$$E(k) = \hbar v_F |\vec{k}|$$

$v_F \sim 10^6 m/s \sim c/300$, good up to $\sim 1ev$

$$H_{\text{Dirac}} = \hbar v_F \begin{bmatrix} \begin{matrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{matrix} & 0 \\ 0 & \begin{matrix} 0 & k_x + ik_y \\ k_x - ik_y & 0 \end{matrix} \end{bmatrix}$$

Massless electrons seen experimentally

Shubnikov-de-Haas oscillations

K. S. Novoselov et. al. *Nature 438, 197 (2005)*

Minimal coupling to magnetic field: $B = \vec{\partial} \times \vec{A}$

$$\vec{\partial} \; \rightarrow \; \vec{D} = \vec{\partial} + i\vec{A}$$

$$H_{\text{Dirac}} = \left[\begin{array}{cc} \begin{array}{cc} 0 & -iD_x - D_y \\ -iD_x + D_y & 0 \end{array} & 0 \\ 0 & \begin{array}{cc} 0 & -iD_x + D_y \\ -iD_x - D_y & 0 \end{array} \end{array} \right]$$

Atiyah-Singer Index Theorem

Number of zero modes $= 2(2) \left| \frac{1}{2\pi} \int d^2 x B(x) \right|$

In the neutral ground state of graphene, half of zero modes are filled. **G. W. S.,** *Phys. Rev. Lett. 53, 2449 (1984)*

Minimal coupling to magnetic field: $B = \vec{\partial} \times \vec{A}$

$$\vec{\partial} \; \rightarrow \; \vec{D} = \vec{\partial} + i\vec{A}$$

$$H_{\rm Dirac} = \begin{bmatrix} \begin{matrix} 0 & -iD_x - D_y \\ -iD_x + D_y & 0 \end{matrix} & 0 \\ 0 & \begin{matrix} 0 & -iD_x + D_y \\ -iD_x - D_y & 0 \end{matrix} \end{bmatrix}$$

Atiyah-Singer Index Theorem

Number of zero modes $= 2(2) \left| \frac{1}{2\pi} \int d^2x B(x) \right|$

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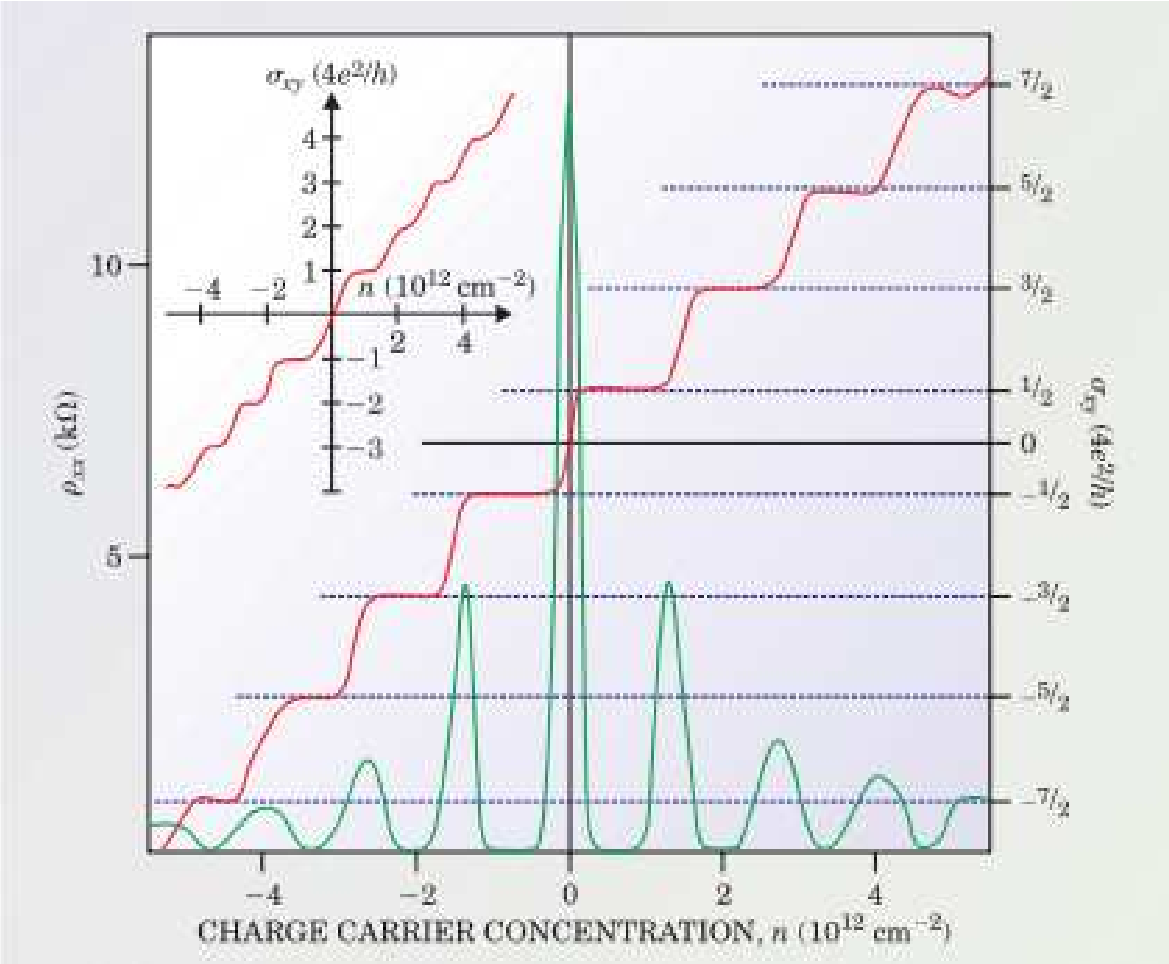
Confirmed by the Quantum Hall Effect in graphene

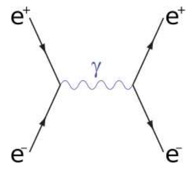
K. Novoselov et. al. *Nature 438, 197 (2005)*

Y. Zhang et. al. *Nature 438, 201 (2005)*



$$\sigma_{xy} = 4\frac{e^2}{h}\left(n + \frac{1}{2}\right)$$

Relativistic Quantum Field Theory



- *"Zitterwebegung"* $\leftrightarrow$ minimum conductivity of graphene $\frac{4e^2}{h}$
- *"Klein paradox"* $\leftrightarrow$ unsuppressed tunneling through barrier
- *"Schwinger effect"* – tunneling production of e^+-e^- pairs by electric field
- *Curvature of space* $\leftrightarrow$ Corrugation of graphene = pseudovector gauge field
- *Dynamical issues* – chiral symmetry breaking
- *Mass condensates* $\longrightarrow$ deformations of graphene lattice $\longrightarrow$ fractionally charged vortices

Graphene for electronic devices

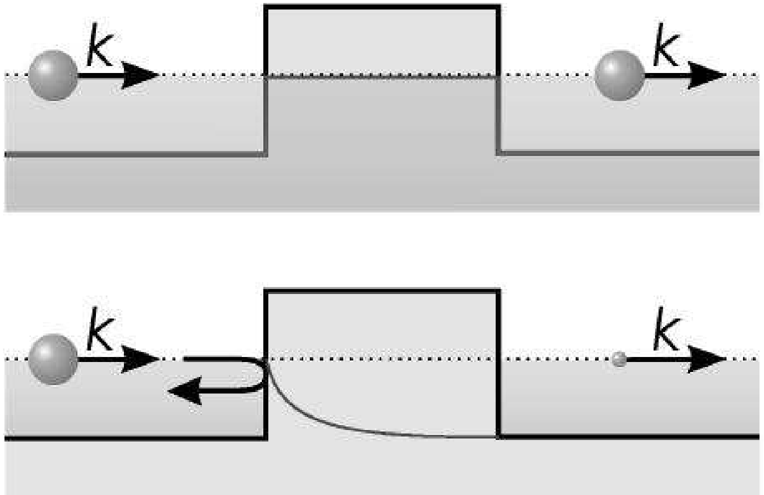
- Graphene has a very large carrier mobility $50,000 cm^2/V s$
- can carry huge current densities $10^8 Amp/cm^2 \ \sim\ 100\times$copper
- Electrons travel ballistically over sales of 1μm.
- Suppressed weak localization (due to corrugations).
- For electronics applications a mass gap is needed (like a conventional semiconductor)

Klein Effect

O. Klein, *Z. Phys. 33, 157 (1929)*

M. Katsnelson, K. S. Novoselov and A. Geim, *Nature Physics 2, 620 (2006)*

Unsuppressed tunneling through a potential barrier



(attempts to observe in QED in collisions of large Z nuclei)

Gapping the spectrum

- Use geometry – graphene quantum dot
- Sublattice symmetry breaking by substrate: deposition on silicon carbide (Lanzara et.al. Berkeley)
- Multi-layer graphene.
- "Graphane"
- Boron-Nitride has same lattice and valence electron dansity but a staggered chemical potential $\mu \sim 4.5ev$ – compare with $t \sim 2.7ev$.
- Graphene layer on top of Boron Nitride. Gap $\sim 50mev$. Lattice constants differ by 1.5 percent.

Gapping the Dirac spectrum in graphene

- parity preserving masses from staggered chemical potential

  G. W. S. *Phys. Rev. Lett. 53, 2449 (1984)*

$$H = \sum_{A,i} \left(t b^{\dagger}_{A+b_i} a_A + t^* a^{\dagger}_A b_{b_A+i} \right) + \mu \sum_A a^{\dagger}_A a_A - \mu \sum_B b^{\dagger}_B b_B$$

  masses of fermion at K and K' points have different signs

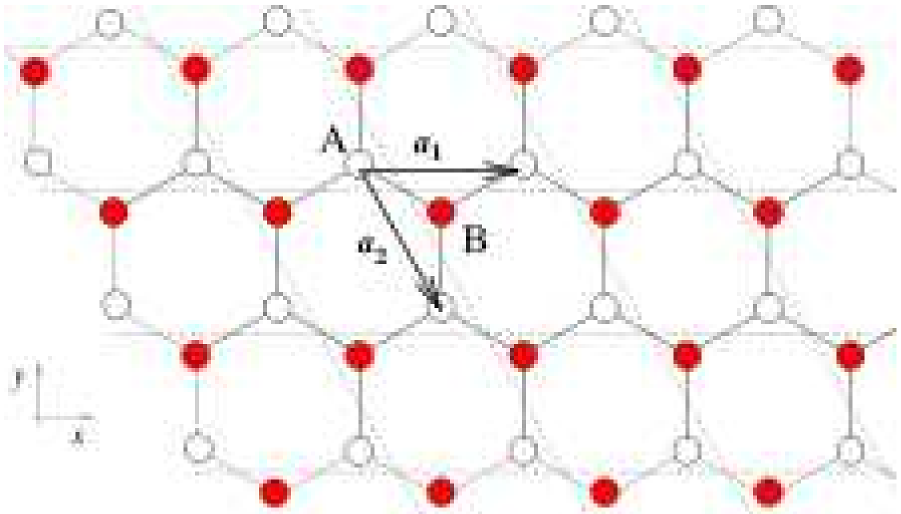
- Other parity preserving mass terms $\sim m\bar{\psi}\gamma^5\psi$ from Kekule lattice distortion

  C. Chamon et. al. *arXiv:0707:0293[cond-mat]*

- Parity violating mass term with external field – masses of K and K' points have same sign – "Hall effect without external field"

  F. D. M. Haldane, *Phys. Rev. Lett. 61, 2015 (1987)*

Mass term from staggered chemical potential:



$$H = \sum_{A,i} \left(t b^\dagger_{A+\vec{b}_i} a_A + t^* a^\dagger_A b_{A+\vec{b}_i} \right) + \mu \sum_A a^\dagger_A a_A - \mu \sum_B b^\dagger_B b_B$$

The resulting Hamiltonian is

$$h = \begin{bmatrix} \mu & t\sum_i e^{i\vec{k}\cdot\vec{a}_i} \\ t^* \sum_i e^{-i\vec{k}\cdot\vec{a}_i} & -\mu \end{bmatrix}$$

Two non-intersecting energy-bands separated by a gap:

$$E(k) = \pm\sqrt{\mu^2 + t^2(1 + 2\cos(\frac{3k_y}{2})\cos(\frac{\sqrt{3}k_x}{2}))^2 + t^2\sin^2(\frac{3k_y}{2})}$$

Linearize near Dirac points $\rightarrow E = \pm\sqrt{\mu^2 + v_F^2 k^2}$

Dirac Hamiltonian for a massive fermion

$$H_{\text{Dirac}} = \begin{bmatrix} \begin{matrix} m & k_x - ik_y \\ k_x + ik_y & -m \end{matrix} & 0 \\ 0 & \begin{matrix} -m & k_x - ik_y \\ k_x + ik_y & m \end{matrix} \end{bmatrix}$$

Two species of massive relativistic fermions that transform into each other under P and T

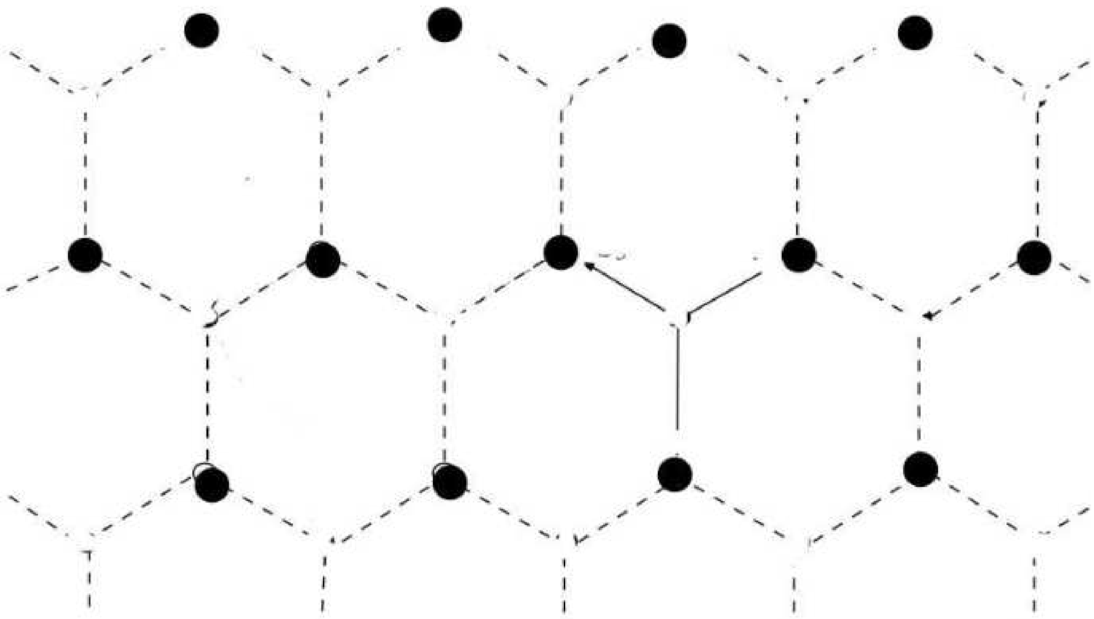
Domain Walls

Consider the electronic properties of omain walls

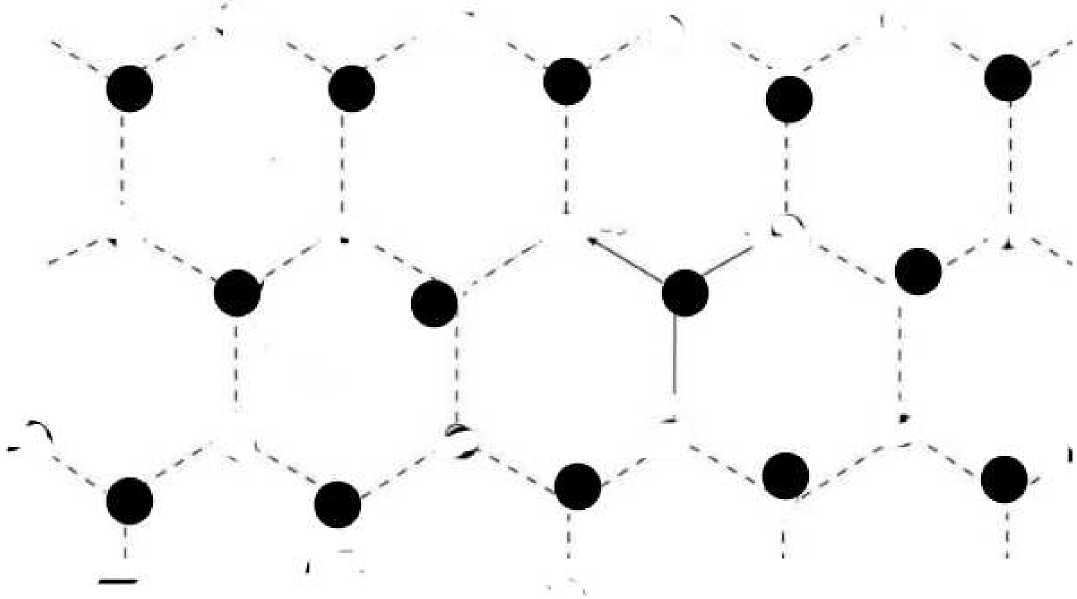
G.W.S. et. al. Phys.Rev.Lett. 101, 087204 (2008)

Virtual Journal of Nanoscale Science & Technology

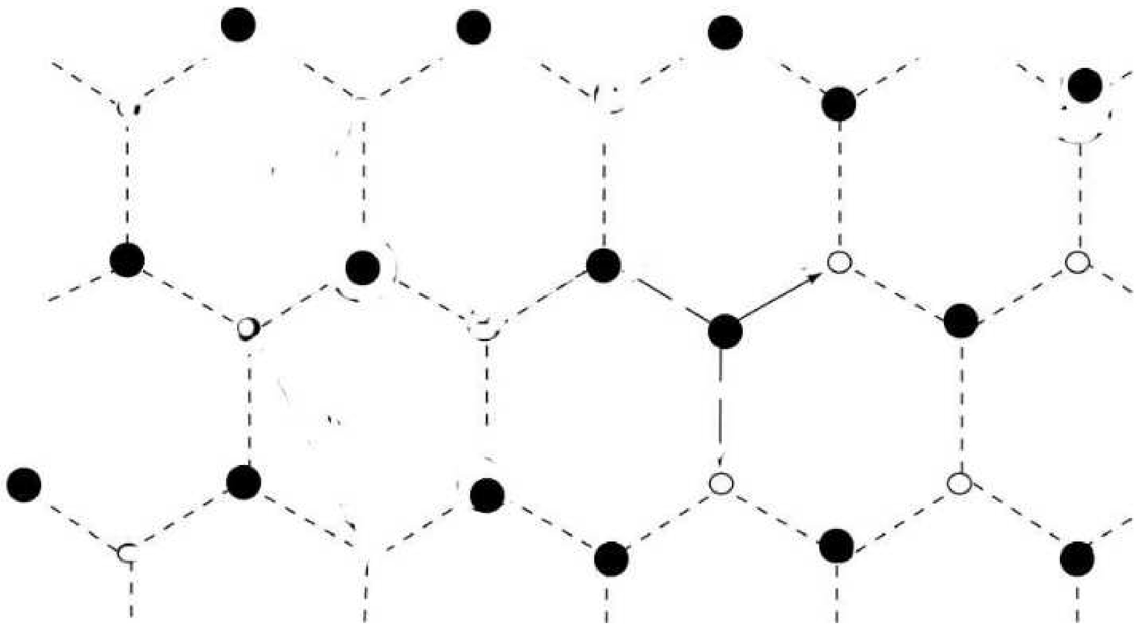
Phase A



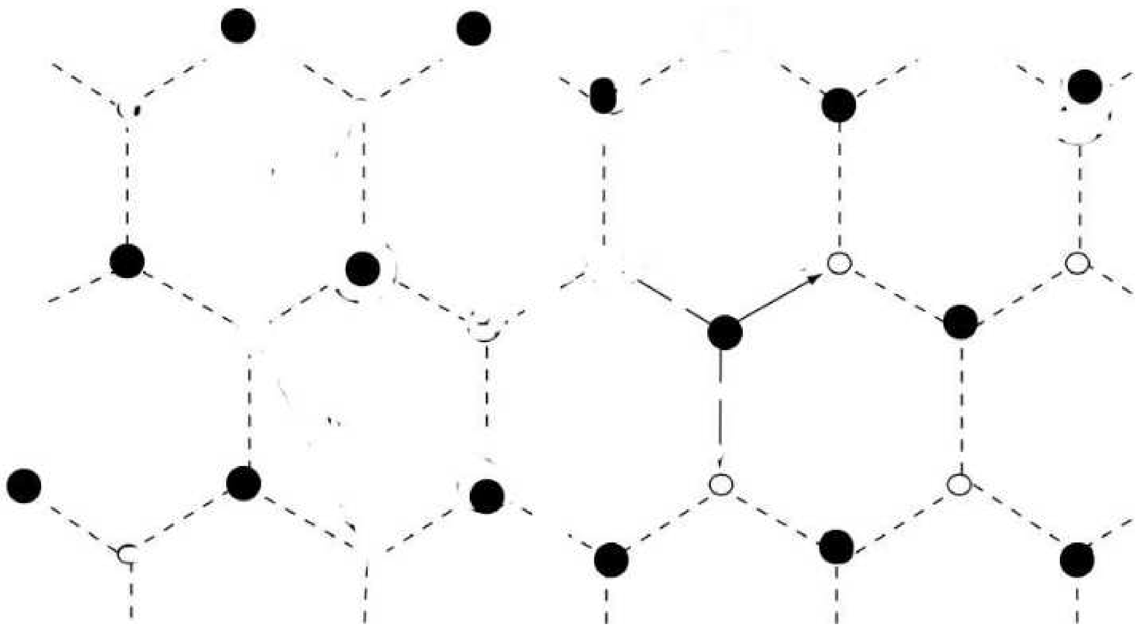
Phase B



Zig-zag Domain Wall Phase A $\rightarrow$ Phase B



Armchair Domain Wall Phase A → Phase B



Domain Wall in the continuum Hamiltonian

In the continuum Hamiltonian the domain wall is described by a position- dependent mass term:

$$H_{\text{Dirac}} = \begin{bmatrix} \begin{matrix} m(x) & -i\partial_x + \partial_y \\ -i\partial_x - \partial_y & -m(x) \end{matrix} & 0 \\ 0 & \begin{matrix} m(x) & -i\partial_x - \partial_y \\ -i\partial_x + \partial_y & -m(x) \end{matrix} \end{bmatrix}$$

where $m(x)$ has a soliton profile

$$m(x \to \infty) = m \quad , \quad m(x \to -\infty) = -m$$

Consider the spinor

$$\psi_L = e^{-iky} \begin{bmatrix} 1 \\ i \\ 0 \\ 0 \end{bmatrix} e^{-\int_0^x dx' m(x')} \quad , \quad \psi_R = e^{-iky} \begin{bmatrix} 0 \\ 0 \\ 1 \\ -i \end{bmatrix} e^{-\int_0^x dx' m(x')}$$

$$H_{\rm Dirac}\,\psi_L(x,y) \;=\; v_F k\,\psi_L(x,y) \;\;,\;\; H_{\rm Dirac}\,\psi_R(x,y) \;=\; -v_F k\,\psi_R(x,y)$$

These are left-movers and right-movers bound to the domain wall.

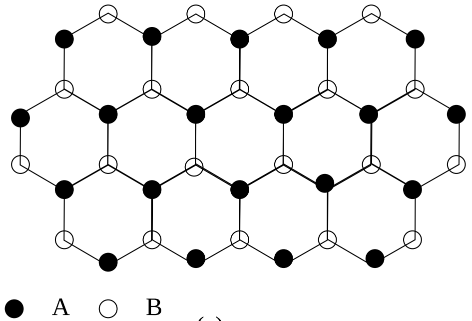
Effective field theory

Massless 1+1-dimensional fermions propagating along the domain wall:

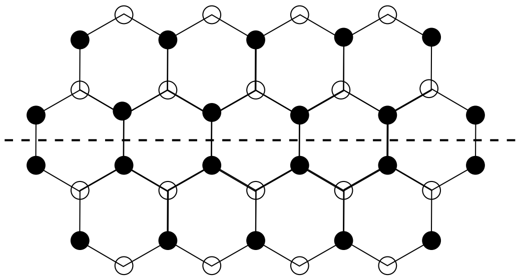
$$H = \hbar v_F \int dy \left(i\psi_L^\dagger \partial_y \psi_L - i\psi_R^\dagger \partial_y \psi_R \right)$$

add interactions = Luttinger liquid or Peierls Instability?

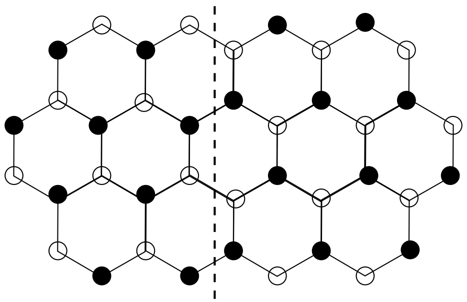
Back to the lattice:



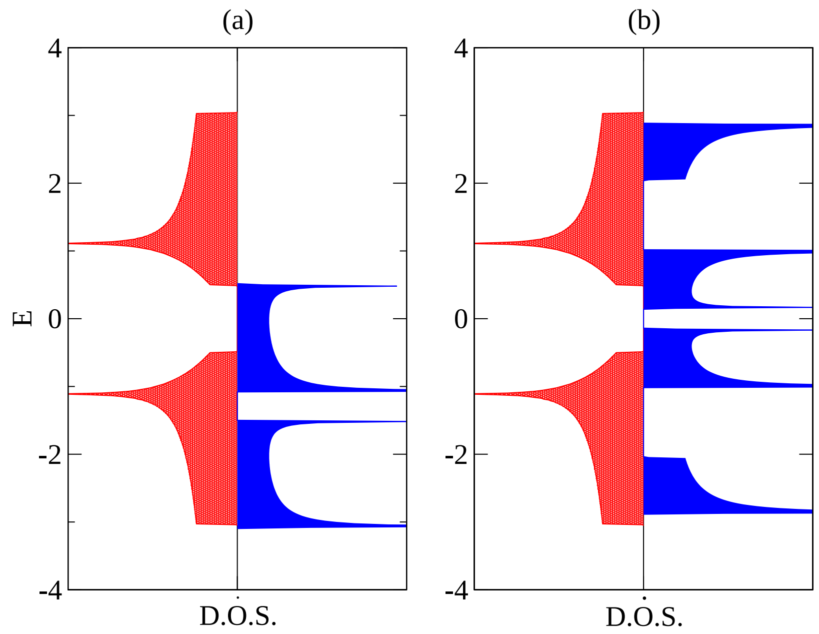
(a)



(b)



(c)

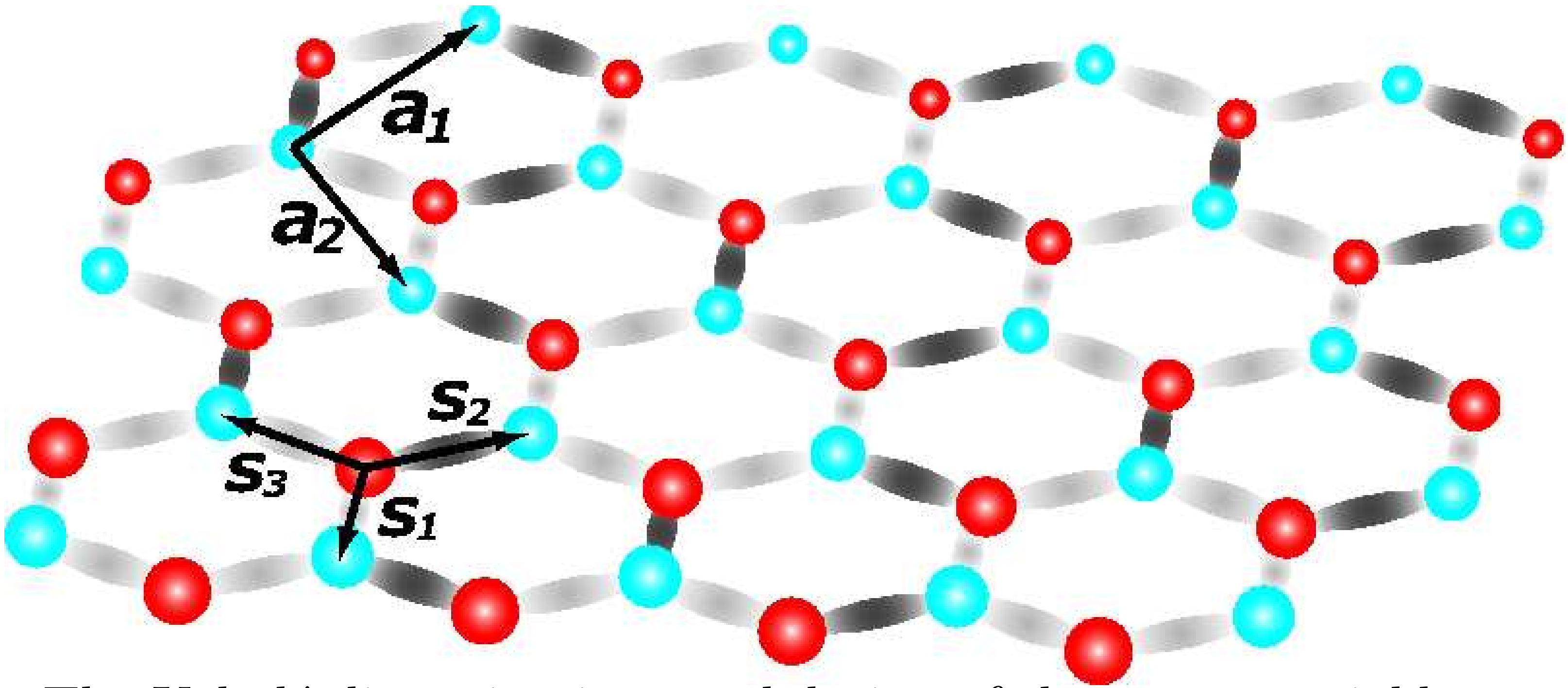


zigzag **armchair**

$$E(k) = t - \sqrt{\mu^2 + 4t^2 \cos^2 \frac{\sqrt{3}a}{2} k_x} \;, \quad E(k) = -t - \sqrt{\mu^2 + 4t^2 \cos^2 \frac{\sqrt{3}a}{2} k_x}$$

Armchair gap $\sim \mu^2/t << \mu$ if $\mu << t$

Kekule distortion



The Kekulé distortion is a modulation of the nearest-neighbor hopping amplitude that is indicated by representing nearest-neighbor bonds of the honeycomb lattice in black (grey) if the hopping amplitude is large (small).

Fractional Charge

The Dirac equation coupled to a mass condensate

$$H_{Dirac} = i\vec{\alpha}\cdot\vec{\nabla} + \beta\ m(x)e^{i\gamma^5\chi(x)}$$

Can have mid-gap states with unpaired helicity.

Charge=$\frac{e}{2}$ per spin degree of freedom.

C. Chamon, C.-Y. Hou, R. Jackiw, C. Mudry, S.Y. Pi and G. W. S., "Electron fractionalization for two-dimensional Dirac fermions", *arXiv:0712.2439 [hep-th]*

Conclusions

- Graphene provides a fascinating laboratory where some otherwise untestable field theory phenomena can be tested.
- Some of these, such as the index theorem, related to the anomalous Hall effect, have already been seen
- Graphene is a promising material for electonic technology.
- Proposals for gapping graphene
- Defects in gapping can have interesting behavior.
- Electric circuits using graphene domain walls?