KIAS-SNU Winter School
4,5 Feb 2010, Pyungchang

Relativistic Dirac Electrons in Solids

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Korea **I**nstitute for **A**dvanced **S**tudy, Seoul, Korea

Outline

Lecture 1. Relativistic Dirac Electrons in Graphene

Lecture 2. Effects of Relativistic Dirac Electrons in Graphene

Lecture 3. Generalizations: Engineering Dirac Electrons

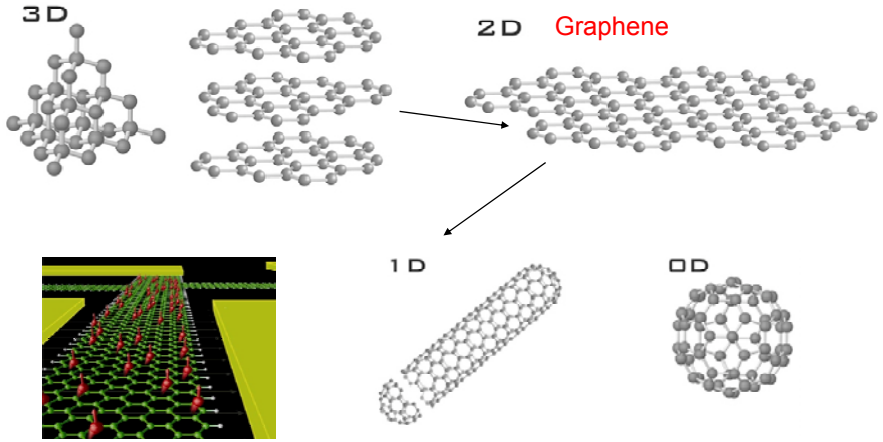
Lecture 4. Relativistic Dirac Electrons in Other Solids
(Quantum Spin Hall Effects and Topological Insulators)

Lecture 1

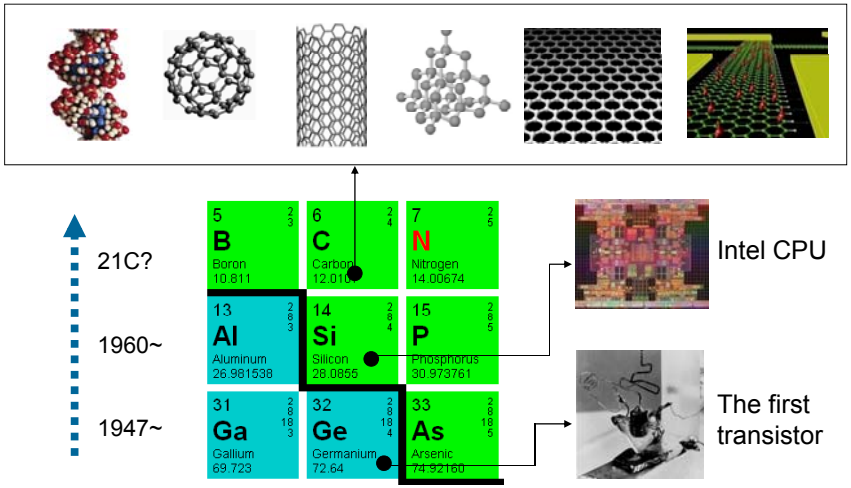
Relativistic Dirac Electrons in Graphene

What is graphene?

- Carbon allotropes



Why Carbon?



This slides is inspired by T. Ohta at LBNL and Fritz-Haber-Institut.

Graphene

- Strongest materials ever measured : Young's modulus 1.0 Tpa
- Thinnest flexible membrane ever created
- Impermeable to gases (even atomic hydrogen)
- Record value for RT thermal conductivity of ~5000 W/mK
- Ballistic transport over micrometers at RT
- Current density six order of magnitude higher than that of Cu
- Room temperature Quantum Hall Effects
- Unique material showing something exotics at RT

Graphene

- Statistics of recent APS March meetings

2009 APS March meeting at Pittsburg, USA

DCMP : Graphene Focus Sessions I-XIX
(Organiziers: A. H. Castro Neto, A. Lanzara, **Y.-W. Son**)

DCMP, DMP, GMAG, FIAP: 9 other sessions

Total 28 Sessions, ~650 talks (960 if including nanotube)
→ ~9% (14%) of total ~7000 talks

✓2007 Denver Meeting 400 (800) talks out of 6800 talks
✓2008 New Orleans Meeting 580 (900) talks out of 6500 talks

Brief history of graphene

- Early works

- Energy bands of graphite calculated

  P. R. Wallace, PR **71**, 622 (47).

- Many important works (Dresselhaus and others)
- Condensed matter analogues to (2+1)D – QED suggested

  G. W. Semenoff, PRL **53**, 2449 (84), E. Fradkin, PRB **33**, 3236 (86), F. D. M. Haldane, PRL **61**, 2015 (88)

- Carbon nanotubes ! (Iijima, 91)
- Single layer of graphene grown on Pt(111) and TiC(111) substrates – CVD of hydrocarbons on metal (promising?)

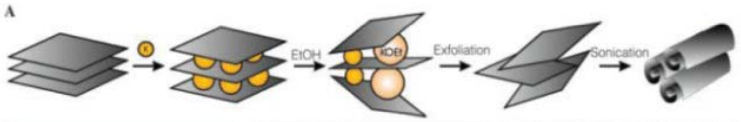
  T. A. Land *et al*, Surf. Sci. **264**, 261 (1992); A. Nagashima *et al*, Surf. Sci. **291**, 93 (1993)

Brief history of graphene

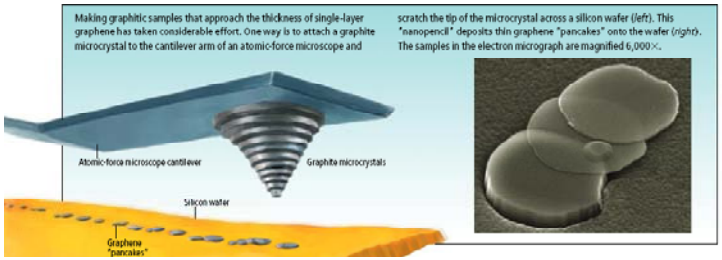
- Early works

- Intercalated graphite as a route to graphene !

L. M. Vicilis *et al*, Science **299**, 1361 (2003).



- Graphene nano-pencil ? (P. Kim@Columbia)



Electronic structure of graphene

- Isolation of graphene ?

VOLUME 61, NUMBER 18 PHYSICAL REVIEW LETTERS 31 OCTOBER 1988

Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"

F. D. M. Haldane
Department of Physics, University of California, San Diego, La Jolla, California 92093
(Received 16 September 1987)

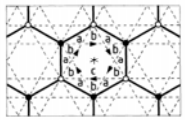


FIG. 1. The honeycomb-net model ("2D graphite") showing nearest-neighbor bonds (solid lines) and second-neighbor bonds (dashed lines). Open and solid points, respectively, mark the *A* and *B* sublattice sites. The Wigner-Seitz unit cell is conveniently centered on the point of sixfold rotation symmetry (marked "*") and is then bounded by the hexagon of nearest-neighbor bonds. Arrows on second-neighbor bonds mark the directions of positive phase hopping in the state with broken time-reversal invariance.

While the particular model presented here is unlikely to be directly physically realizable, it indicates that, at least in principle, the QHE can be placed in the wider context of phenomena associated with broken time-reversal invariance, and does not necessarily require external magnetic fields, but could occur as a consequence of magnetic ordering in a quasi-two-dimensional system.

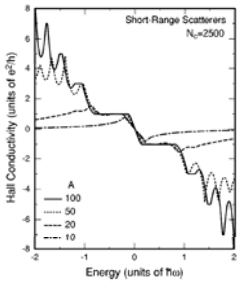
Electronic structure of graphene

- Isolation of graphene ?

PHYSICAL REVIEW B, VOLUME 65, 245420

Hall conductivity of a two-dimensional graphite system

Yisong Zheng* and Tsuneya Ando
Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan
(Received 13 September 2001; revised manuscript received 8 March 2002; published 18 June 2002)



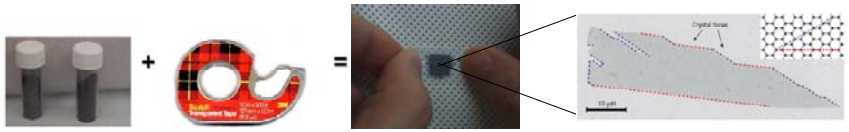
A 2D graphite sheet does not exist in nature. One possible candidate may be graphite intercalation compounds of stage 1 having isolated graphite sheets separated from each other by an intercalant layer. However, the interaction between the graphite layer and intercalants alters the band structure considerably. In fact, most intercalation compounds have Fermi surfaces consisting of a three-dimensional sphere (originating from so-called interlayer states) and that of 2D graphite.[36] Therefore, they do not provide a realistic 2D graphite sheet for the measurement of magnetrotransport.

Exfoliated Graphene

- Breakthrough

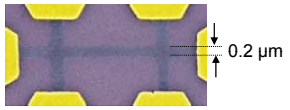
- Micromechanical cleavage of bulk graphite up to 100 micrometer in size via adhesive tapes !

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

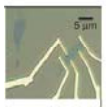


윤두희, 정현식(서강대)

A. K. Geim Group @ Menchester
K. S. Novoselov *et al*, Nature **438**, 197 (2005)



P. Kim Group @ Columbia
Y. Zhang *et al*, Nature **438**, 201 (2005)

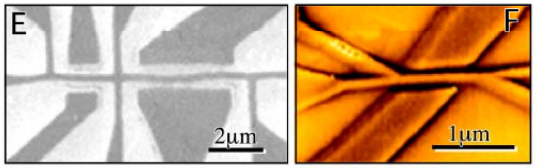


Epitaxial Graphene

- Graphene electronics?

- Epitaxial growth of graphene on SiC{0001}

W. A. de Heer Group at Georgia Tech
C. Berger *et al*, Science **312**, 1191 (2006)



- Precise control of number of layers of graphene
- Large scale graphene productions

CVD Graphene

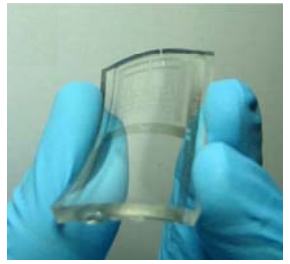
- Graphene electronics?

- Large scale graphene growth by using Chemical Vapor Deposition on thin nickel film and copper foil

Byung Hee Hong group at SKKU
K. S. Kim *et al*, Nature **457**, 706 (2009)

Jing Kong group at MIT
A. Reina *et al*, Nano Lett. **9**, 30 (2009)

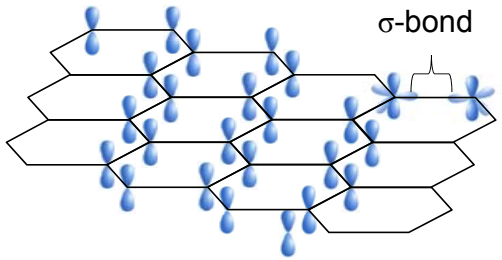
Rod Ruoff group at UT Austin
X. S. Li *et al*, Science **324**, 1312 (2009)



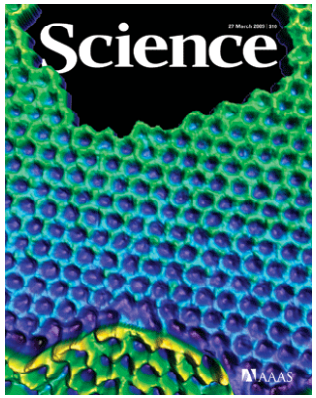
Electronic structure of graphene

- Nature of bonds in graphene

π-orbital



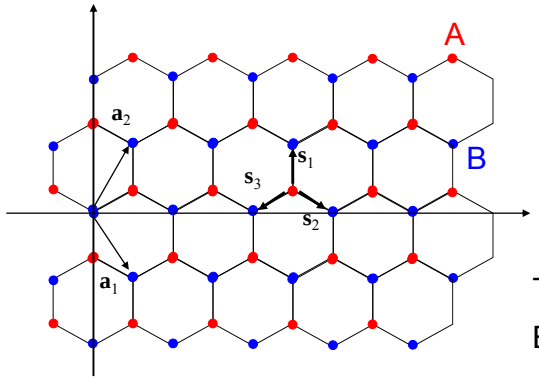
Hexagonal network of Carbon
– sp^2 bonding



TEM image,
Zettl group at UC Berkeley
C. Girit *et al*. Science **323**, 170 (2009)

Electronic structure of graphene

- Real space: tight-binding Hamiltonian



Two sublattices -
Bipartite system

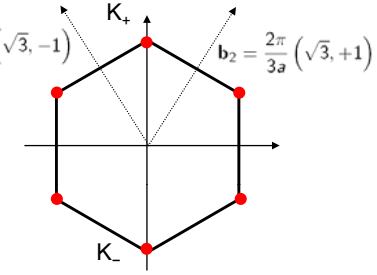
Nearest-neighbor tight-binding Hamiltonian for π-orbitals

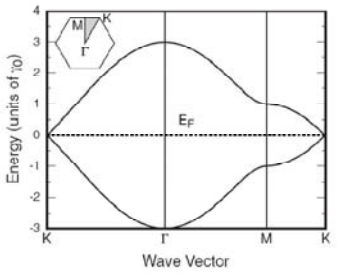
$$\mathcal{H} = -t \sum_{\mathbf{r}\in A} \sum_{i=1,2,3} \left[a^\dagger(\mathbf{r}) b(\mathbf{r}+\mathbf{s}_i) + b^\dagger(\mathbf{r}+\mathbf{s}_i) a(\mathbf{r}) \right]$$

Electronic structure of graphene

- Energy spectrum

$$\mathbf{b}_1 = \frac{2\pi}{3a}\left(\sqrt{3}, -1\right) \qquad \mathbf{b}_2 = \frac{2\pi}{3a}\left(\sqrt{3}, +1\right)$$





$$\mathcal{H} = \sum_{\mathbf{k}} \left[\Phi(\mathbf{k}) a^\dagger(\mathbf{k}) b(\mathbf{k}) + \Phi^*(\mathbf{k}) b^\dagger(\mathbf{k}) a(\mathbf{k})\right]$$

$$= \sum_{\mathbf{k}} \left(a^\dagger(\mathbf{k}) \quad b^\dagger(\mathbf{k})\right) \begin{pmatrix} 0 & \Phi(\mathbf{k}) \\ \Phi^*(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} a(\mathbf{k}) \\ b(\mathbf{k}) \end{pmatrix}$$

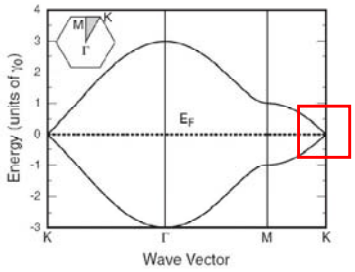
$$\mathcal{E}(\mathbf{k}) = \pm t\,|\Phi(\mathbf{k})| = \pm t \left|1 + 2e^{-i\frac{3}{2}k_y} \cos\left(\frac{\sqrt{3}}{2}k_x\right)\right|$$

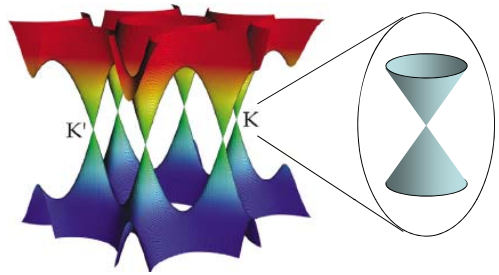
- Hexagonal BZ with two special Fermi points,

$$\mathbf{K}_\pm = \left(\pm\frac{4\pi}{3\sqrt{3}a}, 0\right)$$

Electronic structure of graphene

- Linear energy bands





- Two inequivalent Dirac cones at K and K'

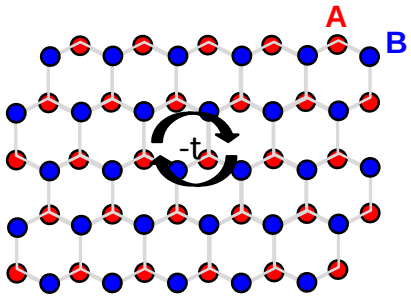
$$\Phi_+(\mathbf{p}) = -t \sum_{j=1,2,3} e^{-i(\mathbf{K}_+ + \mathbf{p})\cdot\mathbf{s}_j}$$

$$\simeq t \sum_{j=1,2,3} e^{-i\mathbf{K}_+\cdot\mathbf{s}_j} (i\mathbf{p}\cdot\mathbf{s}_j)$$

$$= \frac{3at}{2}(p_x - ip_y) = v_F(p_x - ip_y)$$

Electronic structure of graphene

- Real space



$$e^{-i\frac{\theta_p}{2}} H\left(\frac{1}{\hbar}\right) = v_F \sum_{\mathbf{k}} \sum_{\langle i,j\rangle} \left(c_A^\dagger(\mathbf{k}) \; c_B^\dagger(\mathbf{k})\right) \begin{pmatrix} 0 & \Phi(\mathbf{k}) \\ \Phi^*(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} c_A(\mathbf{k}) \\ c_B(\mathbf{k}) \end{pmatrix}$$

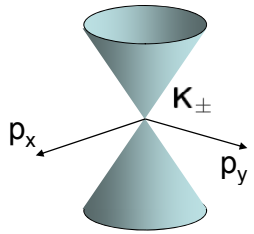
(Pseudo) two-component wavefunctions

(Pseudo) Dirac Hamiltonian

$$H = v_F \sum_{\mathbf{p}} \left(c_A^\dagger(\mathbf{p}) \; c_B^\dagger(\mathbf{p})\right) \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} \begin{pmatrix} c_A(\mathbf{p}) \\ c_B(\mathbf{p}) \end{pmatrix}$$

Electronic structure of graphene

- 'Neutrino' in your pencil?



$$H = v_F\left(\sigma_x p_x + \sigma_y p_y\right) = v_F \boldsymbol{\sigma}\cdot\mathbf{p}$$

Dirac equation with zero mass

→ charged 'neutrino' in your pencil?

- Relativistic particle :

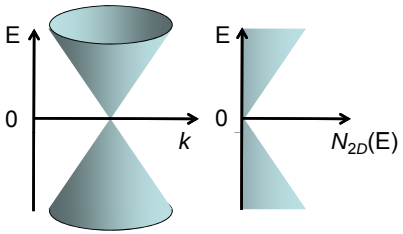
$$E = \pm\sqrt{c^2p^2 + m^2c^4} = \pm v_F|\mathbf{p}|$$

c=v_F: effective speed of 'light' m=0

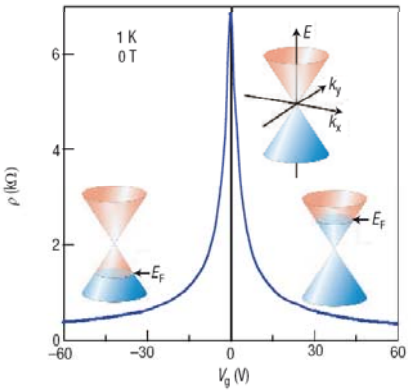
Electronic structure of graphene

- Consequences of massless Dirac fermions

Linear Density of States



$$\rho_{max} \sim \frac{h}{4e^2}$$



$$\rightarrow \rho = \frac{1}{e^2 v_F l_e N_{2D}(E)}$$

Zhang *et al*, Novoselov *et al* (05)

Transport properties of graphene

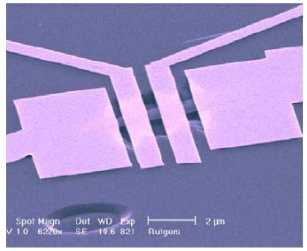
- Mobility of graphene

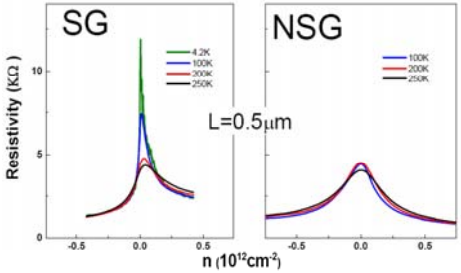
Mobility of suspended graphene ~ 200,000 cm^2/Vs

Observation of nearly ballistic transport regime/ FQHE

X. Du *et al*, Nature Nanotech. **3**, 491 (2008).
K. I. Botolin *et al*. SSC **146**, 351 (2008)

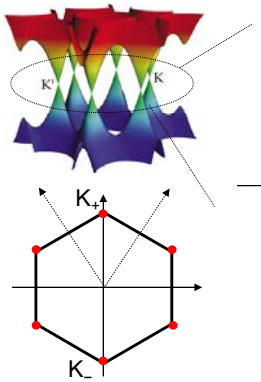
X. Du *et al*, Nature **462**, 192 (2009).
K. I. Botolin *et al*. Nature **462**, 196 (2009)

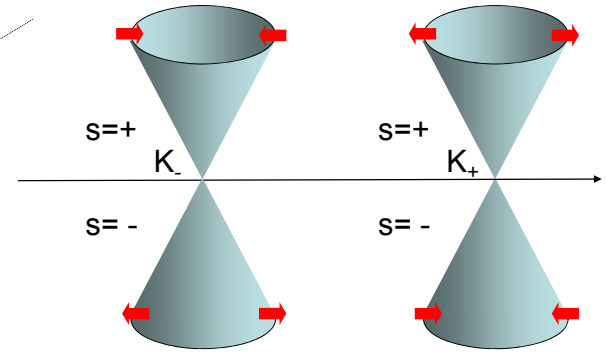




Electronic structure of graphene

- Total Hamiltonian





$$\rightarrow \mathcal{H}_{tot}(\mathbf{p}) = v_F\left[p_x(\sigma_x \otimes \tau_z) + p_y(\sigma_y \otimes \mathbf{1}_2)\right] \text{ with } \Psi = \begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix}$$

σ acts on sublattice A (B) and τ on K_+ (K_-)

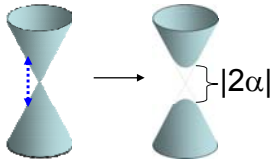
Electronic structure of graphene

- Gap generation in graphene

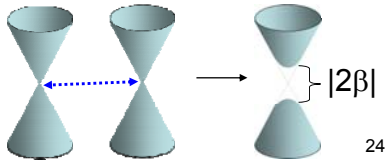
$$\mathcal{H} = \begin{array}{c} \begin{matrix} KA & KB & K'A & K'B \end{matrix} \\ \begin{pmatrix} \alpha & v_F(\hat{k}_x - i\hat{k}_y) & 0 & \beta \\ v_F(\hat{k}_x + i\hat{k}_y) & -\alpha & \beta & 0 \\ 0 & \beta^* & \alpha & -v_F(\hat{k}_x + i\hat{k}_y) \\ \beta^* & 0 & -v_F(\hat{k}_x - i\hat{k}_y) & -\alpha \end{pmatrix} \end{array}$$

$$\rightarrow E = \pm\sqrt{v_F^2 k^2 + |\alpha|^2 + |\beta|^2}$$

Onsite energy difference
- Mixing pseudo-spins



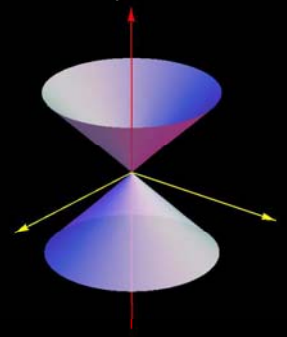
Mixing between K_+ and K_-
- Mixing chiralities



Electronic structure of graphene

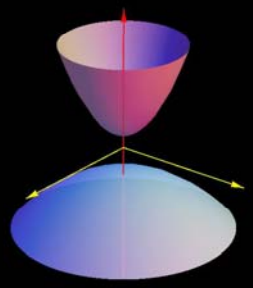
- Low energy dispersions

Graphene



$H = v_F(\sigma_x p_x + \sigma_y p_y) = v_F \boldsymbol{\sigma} \cdot \boldsymbol{p}$

Usual Semiconductor

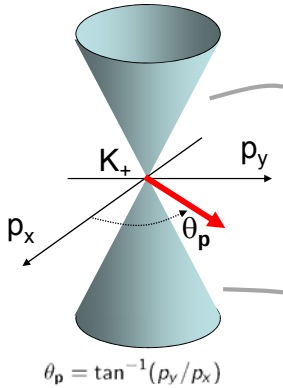


$H = \frac{p^2}{2m} + V(r)$

Electronic structure of graphene

- Pseudospin and chiral states

$$H = v_F(\sigma_x p_x + \sigma_y p_y) = v_F \boldsymbol{\sigma} \cdot \mathbf{p}$$



Eigenfunctions : Spinor representation

$$\psi_c = e^{-i\frac{\theta_p}{2}}\begin{pmatrix}1\\0\end{pmatrix} + e^{+i\frac{\theta_p}{2}}\begin{pmatrix}0\\1\end{pmatrix}$$

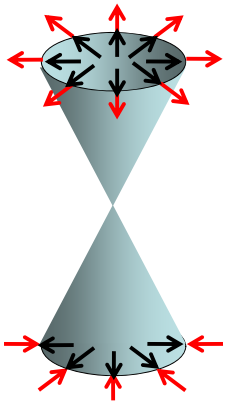
$$= e^{-i\frac{\theta_p}{2}}|\uparrow\rangle + e^{+i\frac{\theta_p}{2}}|\downarrow\rangle$$

$$\psi_v = e^{-i\frac{\theta_p}{2}}|\uparrow\rangle - e^{+i\frac{\theta_p}{2}}|\downarrow\rangle$$

Pseudo-spin up (down): A (B) sublattice

Electronic structure of graphene

- Chiral states: charged "*neutrino*" in your pencil



Helicity operator : $\hat{h} = \frac{1}{2}\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}$

• Conduction band :

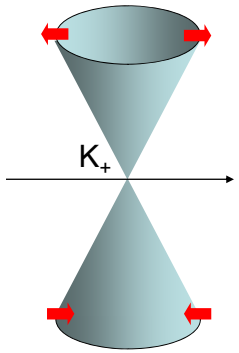
$$\hat{h}\,\psi_c = \frac{1}{2}\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}\,\psi_c = \frac{1}{2}\psi_c$$

σ_x = -1/2 ← (-e) → σ_x = +1/2

$p_x < 0$ ← → $p_x > 0$

Electronic structure of graphene

- Consequence of chirality



• Eigenstates :

$$\langle \mathbf{r}|s\mathbf{p},+\rangle = \Psi_{s\mathbf{p},+}(\mathbf{r}) = \frac{1}{\sqrt{2}} e^{i\mathbf{p}\cdot\mathbf{r}} R^{-1}(\theta_p)\begin{pmatrix}1\\s\end{pmatrix}$$

• For a long-range disorder where $|\mathbf{q}| \ll K$ a elastic scattering matrix element is

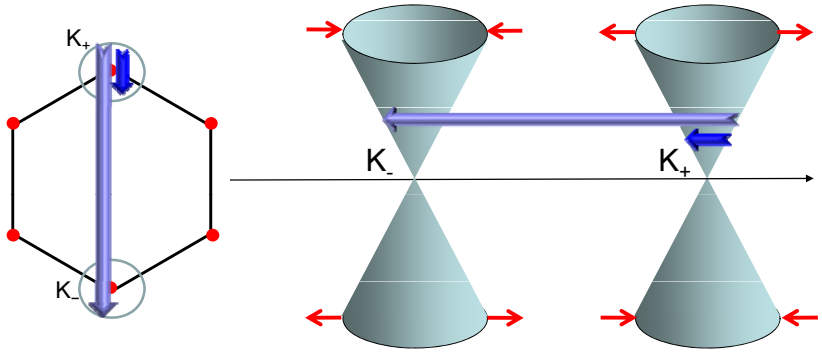
$$|\langle s\mathbf{p}'|V|s\mathbf{p}\rangle|^2 = |V(\mathbf{p}'-\mathbf{p})|^2 \cos^2\left(\frac{\theta_p - \theta_{p'}}{2}\right)$$

: Complete absence of backscattering (pseudospin conservation)

• Klein paradox: M. I. Katsnelson *et al*, Nature Phys. **2**, 620 (2006)

• Veselago lens: V. V. Cheianov *et al*, Science **315**, 1252 (2007)

Electronic structure of graphene
- Scattering

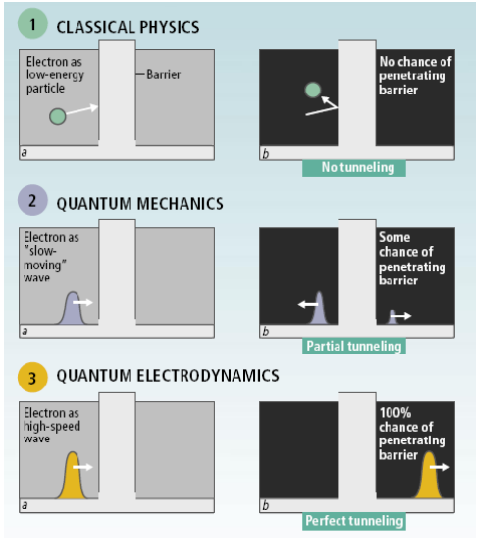


- Intra-valley scattering: small momentum transfer, lattice distortion, etc.
- Inter-valley scattering: large momentum transfer, short range atomic impurities, etc

Lecture 2

Consequences

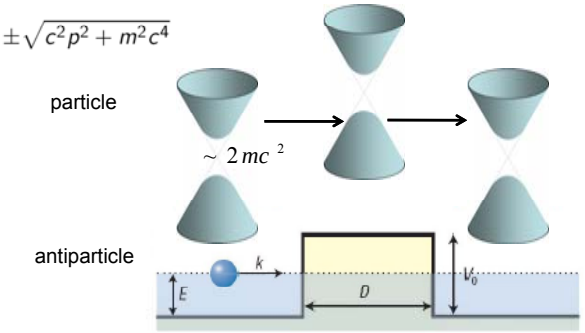
Electronic structure of graphene
- Tunneling



A. K. Geim & P. Kim Scientific American, Apr. 2008

Electronic structure of graphene
- Klein paradox

$E = \pm\sqrt{c^2p^2 + m^2c^4}$

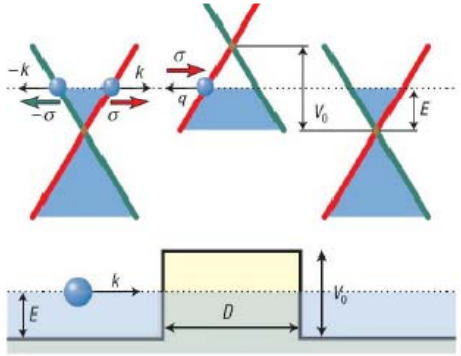


- Klein paradox: Unimpeded penetration of relativistic particles through very high potential barriers.
- Potential drop $\sim 2mc^2$ over $\hbar/mc$: ~10^8 V/Å
  - → Event horizon of Black hole
  - → Supercritical massive atoms

O. Klein, Z. Phys. **53**, 157 (1929)

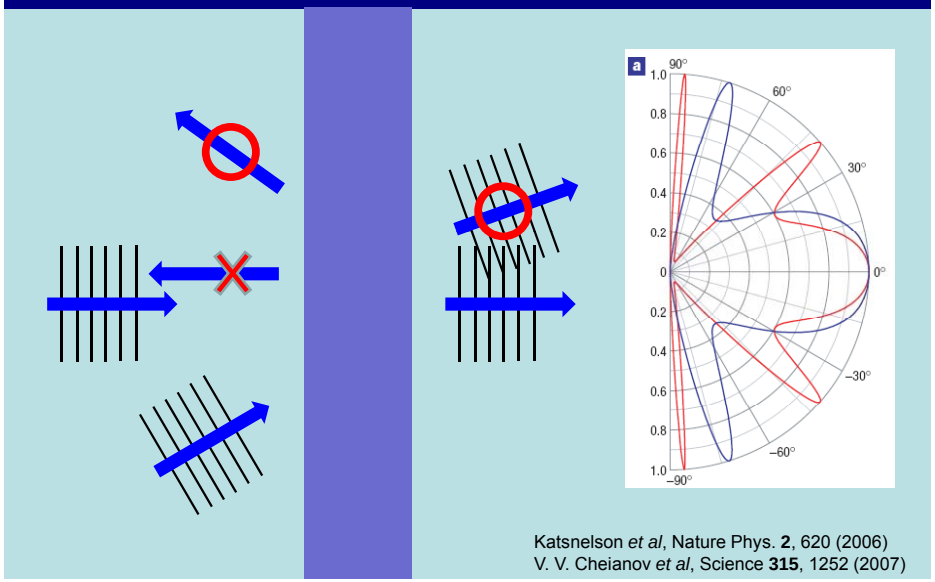
Electronic structure of graphene
- Klein tunneling

Graphene



Katsnelson *et al*, Nature Phys. **2**, 620 (2006)
V. V. Cheianov *et al*, Science **315**, 1252 (2007)
…
C. Park, **Y.-W. Son** *et al*, Nature Phys. (2008),
Phys. Rev. Lett. (2008),
Nano Lett (2008)

Electronic structure of graphene
- Klein tunneling



Katsnelson *et al*, Nature Phys. **2**, 620 (2006)
V. V. Cheianov *et al*, Science **315**, 1252 (2007)

Transport properties of graphene
- Klein tunneling

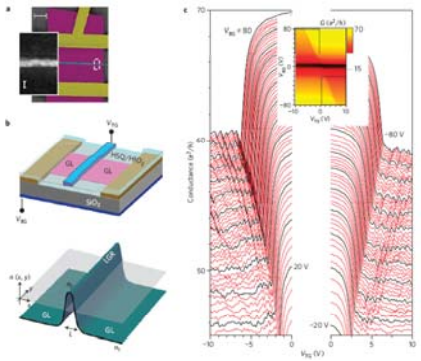
LETTERS
PUBLISHED ONLINE: 1 FEBRUARY 2009 | DOI: 10.1038/NPHYS1198
nature physics

Quantum interference and Klein tunnelling in graphene heterojunctions

Andrea F. Young and Philip Kim*

Pabry-Ferot interference: observation of Berry's phase

A. F. Young & P. Kim, Nature Phys. **5**, 222 (2009).
N. Stander, B. Huard, D. Goldhaber-Gordon,
Phys. Rev. Lett. **102**, 026807 (2009)

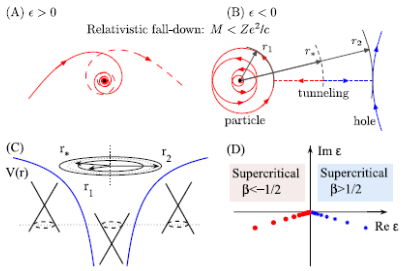


Electronic structure of graphene
- Klein paradox

PRL 99, 246802 (2007) PHYSICAL REVIEW LETTERS week ending 14 DECEMBER 2007

Atomic Collapse and Quasi–Rydberg States in Graphene

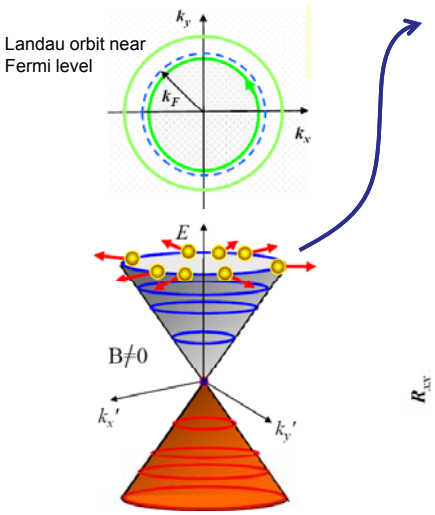
A. V. Shytov,[1] M. I. Katsnelson,[2] and L. S. Levitov[3]
[1]*Brookhaven National Laboratory, Upton, New York 11973-5000, USA*
[2]*Radboud University of Nijmegen, Toernooiveld 1 6525 ED Nijmegen, The Netherlands*
[3]*Department of Physics, Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, Massachusetts 02139, USA*
(Received 6 August 2007; published 14 December 2007)



- Supercritical atomic collapse if $Z \geq 137$
- In graphene, divalent or trivalent impurities e.g. Ca, Yb, La, Gd are enough to realize this effect.

Electronic structure of graphene

- Shubnikov-de Hass Oscillation and Berry's phase

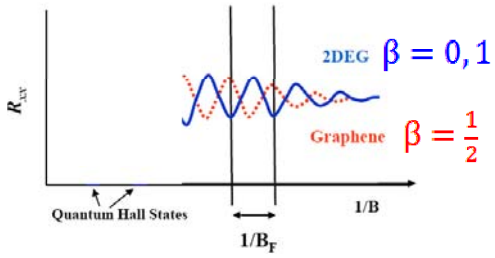


$$\psi(\boldsymbol{p}) = R^{-1}(\theta_p)\begin{pmatrix}1\\1\end{pmatrix}$$

$$R(\theta_p) = \exp\left(i\frac{\theta_p}{2}\sigma_z\right) \qquad \hat{p}_x + i\hat{p}_y = e^{i\theta_p}$$

$$R(\theta_p \pm 2\pi) = -R(\theta_p)$$

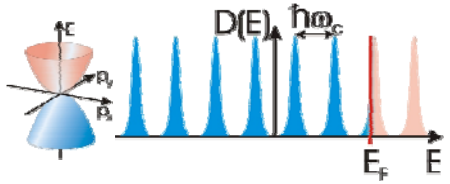
$$\Delta R_{xx} = -R(B,T)\cos\left(2\pi\frac{B_F}{B} + 2\pi\beta\right)$$



Electronic structure of graphene

- Landau levels in perpendicular B-field

Parabolic band (normal metal)

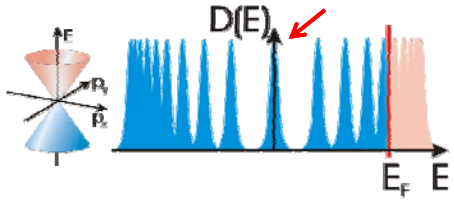


$$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right)$$

$$\omega_c = \frac{eB}{mc} = \frac{\hbar}{ml_B^2}, \quad l_B = \sqrt{\frac{\hbar c}{eB}}$$

$$B = 10\,T, \quad \hbar\omega_c \approx 1K$$

Linear band (single layer graphene)



$$E_n = \hbar\omega_c\sqrt{n}$$

$$\omega_c = \frac{v_F}{l_B} = v_F\sqrt{\frac{eB}{\hbar c}}$$

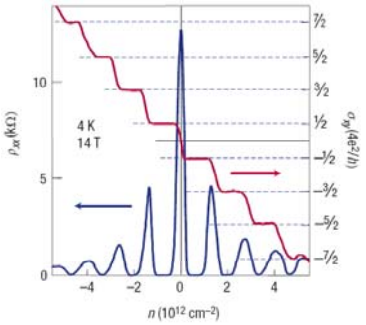
$$B = 10\,T, \quad \hbar\omega_c \approx 1500K$$

Electronic structure of graphene

- Consequences of chiral massless Dirac fermions

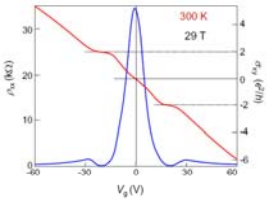
Half-integer Quantum Hall Effect (Room T) !

(Manifestation of Berry's phase of pseudospin)



Zhang *et al* (05), Novoselov *et al* (05)

Kim & Geim *et al* (07)



$$R_{xy}^{-1} = \pm g_s \cdot (\nu + \frac{1}{2}) \cdot \frac{e^2}{h}$$

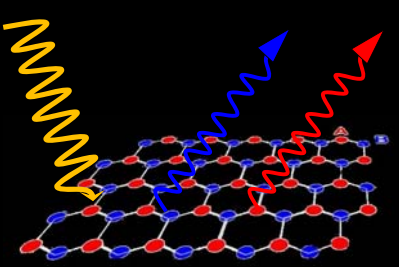
$$\nu = 1, 2, 3, \cdots$$

$$g_s = 2 \times 2 \text{ (spin \& sublattice)}$$

Haldane (88), T. Ando (02)

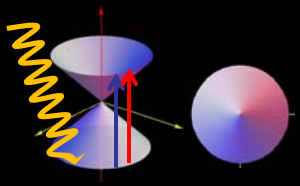
Electronic structure of graphene

- Consequence of chiral massless Dirac particles

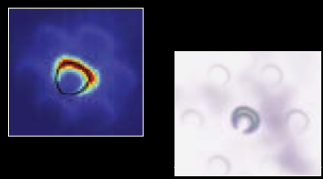


Photoemission experiments :
Crescent shape anisotropy
(*à la* Young's double slit !)

$$I \sim \left|e^{+i\frac{\theta}{2}} + e^{-i\frac{\theta}{2}}\right|^2 \sim \cos^2\frac{\theta}{2}$$



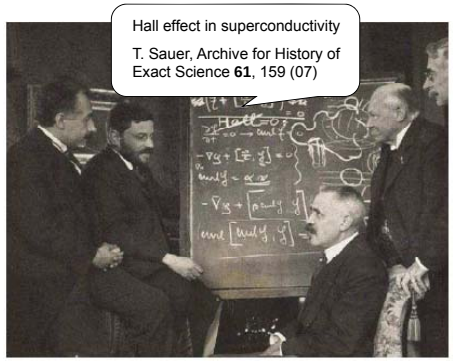
Bostwick *et al*, Nature Phys **3**, 36 (07)
Zhou *et al*, Nature Mat **6**, 770 (07)

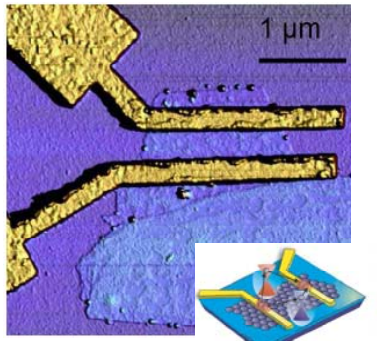


Kim, Ihm, Choi & **Son**,
arXiv.org:*0912.1210* (09)

Electronic structure of graphene

- Special relativity vs Superconductivity





Oct. 1920 Leiden, Einstein, Ehrenfest, Langevin, Onnes

H. B. Heersche, P. Jarillo-Herrero *et al*, Nature **446**, 56 (2007)

Electronic structure of graphene

- Gap?

Fine structure constant, $\alpha = \frac{e^2}{\hbar c} \simeq \frac{1}{137}$

"Effective Fine structure constant" in graphene : $\alpha_G = \frac{e^2}{\varepsilon \hbar v_F} \simeq \frac{300}{137 \times \varepsilon}$

PRL **102,** 026802 (2009) PHYSICAL REVIEW LETTERS week ending 16 JANUARY 2009

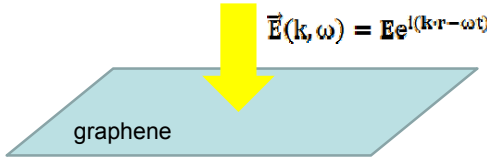
Is Graphene in Vacuum an Insulator?

Joaquín E. Drut[1] and Timo A. Lähde[2]
[1]*Department of Physics, The Ohio State University, Columbus, Ohio 43210-1117, USA*
[2]*Department of Physics, University of Washington, Seattle, Washington 98195-1560, USA*
(Received 11 July 2008; published 13 January 2009)

We present evidence, from lattice Monte Carlo simulations of the phase diagram of graphene as a function of the Coulomb coupling between quasiparticles, that graphene in vacuum is likely to be an insulator. We find a semimetal-insulator transition at $\alpha_g^{\text{crit}} = 1.11 \pm 0.06$, where $\alpha_g \simeq 2.16$ in vacuum, and $\alpha_g \simeq 0.79$ on a SiO_2 substrate. Our analysis uses the logarithmic derivative of the order parameter, supplemented by an equation of state. The insulating phase disappears above a critical number of four-component fermion flavors $4 < N_f^{\text{crit}} < 6$. Our data are consistent with a second-order transition.

Electronic structure of graphene

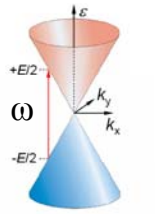
- Opacity



$$\vec{E}(k,\omega) = Ee^{i(k\cdot r-\omega t)}$$

$$H = v_F\vec{\sigma}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right) = H_0 + H_{int}$$

$$H_{int} = v_F\vec{\sigma}\cdot\frac{e}{c}\vec{A} = v_F\vec{\sigma}\cdot\frac{e}{i\omega}\vec{E}$$



$$P(\text{absorption}) = \frac{W_a}{W_i} = \frac{\text{absorbed energy by graphene}}{\text{incident energy}}$$

$$W_i = \frac{c}{4\pi}|\vec{E}|^2$$

$$W_a = \frac{2\pi}{\hbar}|M|^2 D\left(\frac{\hbar\omega}{2}\right)\times\hbar\omega$$

$$D\left(\frac{\hbar\omega}{2}\right) = \frac{\hbar\omega}{\pi\hbar^2 v_F^2}$$

$$|M|^2 = \left|\langle\psi_f|v_F\vec{\sigma}\cdot\frac{e}{i\omega}\vec{E}|\psi_i\rangle\right|^2 = \frac{1}{8}e^2v_F^2\frac{|\vec{E}|^2}{\omega^2}$$

$$P(\text{absorption}) = \frac{W_a}{W_i} = \frac{(e^2/4\hbar)|\vec{E}|^2}{(c/4\pi)|\vec{E}|^2} = \frac{\pi e^2}{\hbar c} = \pi\alpha$$

Electronic structure of graphene

- Opacity

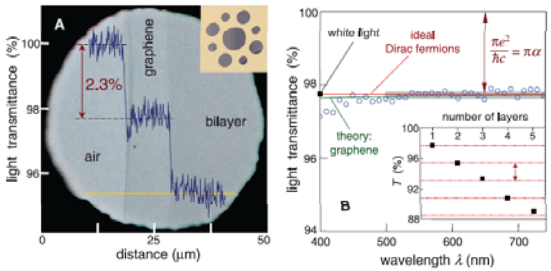
$$P(\text{absorption}) = \frac{W_a}{W_i} = \frac{(e^2/4\hbar)|\vec{E}|^2}{(c/4\pi)|\vec{E}|^2} = \frac{\pi e^2}{\hbar c} = \pi\alpha$$

Fine Structure Constant Defines Visual Transparency of Graphene

R. R. Nair,[1] P. Blake,[1] A. N. Grigorenko,[1] K. S. Novoselov,[1] T. J. Booth,[1] T. Stauber,[2] N. M. R. Peres,[2] A. K. Geim[1]*

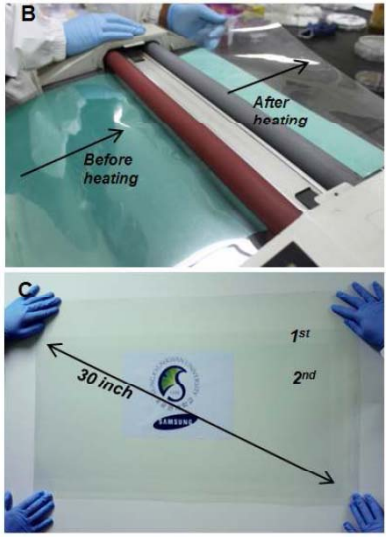
Science **320**, 1308 (2008)

Transmittance ~ 97.7%



Electronic structure of graphene

- Opacity



Materials	Fracture Strain	Materials	Fracture Strain
Silicon	~ 0.7%	Poly- ZnO	0.03%
ITO	0.58 ~ 1.15%	Polyimide	4%
Au	0.46%	CNT, Graphene	~ 20%

- Transparent flexible display?
- Replacement of ITO?

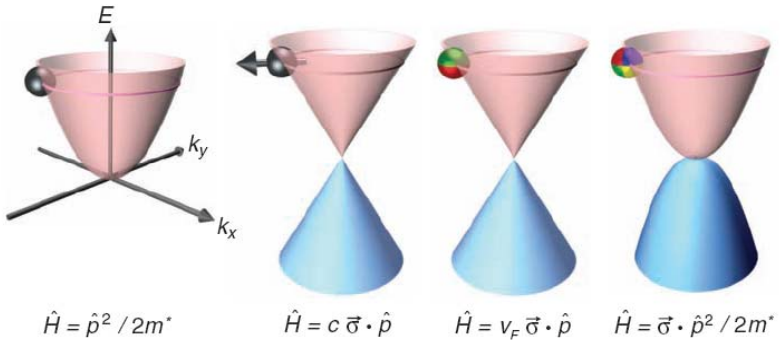
- Prof. Byung Hee Hong (SKKU) arXiv.org:0912.5485

See Video >>>

Lecture 2

Bilayer Graphene

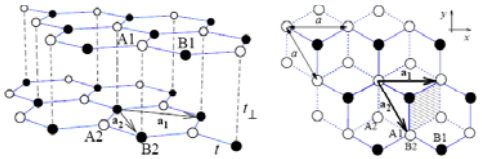
What is bilayer graphene?



Normal material | Neutrino | Graphene | Bilayer Graphene

- Only single layer graphene has a linear dispersion.
- All others are massive, i.e., almost normal metals But,

Bilayer graphene
: Massive chiral particles



Minimal model: Two coupled single layer graphene with dimer couplings A1-B2

$$\mathcal{H} = \begin{pmatrix} 0 & v_F\pi & 0 & 0 \\ v_F\pi^\dagger & 0 & t_\perp & 0 \\ 0 & t_\perp & 0 & v_F\pi \\ 0 & 0 & v_F\pi^\dagger & 0 \end{pmatrix}$$

$$\pi = p_x - ip_y = |\mathbf{p}|e^{-i\phi_{\mathbf{p}}}$$

$$\Psi = (\psi_{B_1}, \psi_{A_1}, \psi_{B_2}, \psi_{A_2})^T$$

Bilayer graphene
: Massive chiral particles

Bilayer Graphene

Low energy effective Hamiltonian by integrating out high energy dimer part

$$\mathcal{H}_{\text{eff}} \simeq \frac{v_F^2}{t_\perp}\begin{pmatrix} 0 & \pi^2 \\ (\pi^\dagger)^2 & 0 \end{pmatrix} = \frac{|\mathbf{p}|^2}{2m^*}\vec{\sigma}\cdot\hat{n}_{\mathbf{p}} \qquad m^* = \frac{t_\perp}{2v_F^2}$$

MASSIVE CHIRAL

$$\hat{n}_{\mathbf{p}} = (\cos(2\phi_{\mathbf{p}}), \sin(2\phi_{\mathbf{p}}))$$

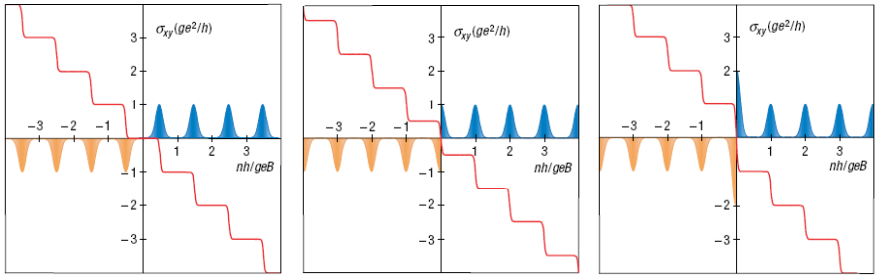
Single layer Graphene

$$\mathcal{H}_{\text{eff}} \simeq v_F\begin{pmatrix} 0 & \pi \\ \pi^\dagger & 0 \end{pmatrix} = v_F|\mathbf{p}|\vec{\sigma}\cdot\hat{n}_{\mathbf{p}} \qquad \hat{n}_{\mathbf{p}} = (\cos(1\phi_{\mathbf{p}}), \sin(1\phi_{\mathbf{p}}))$$

MASSLESS CHIRAL

Bilayer graphene
: Massive chiral particles

Normal Metal	Single layer Graphene	Bilayer Graphene

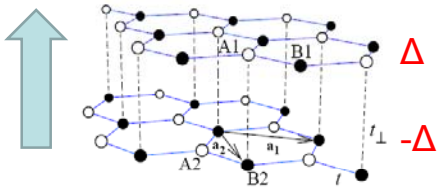


$$E_N = \hbar\omega_c\left(N+\frac{1}{2}\right) \qquad E_N = \pm\hbar\omega_c\sqrt{N} \qquad E_N = \pm\hbar\omega_c\sqrt{N(N-1)}$$

$$\sigma_{xy} = \pm\frac{4e^2}{h}N\ (N \geq 0) \qquad \sigma_{xy} = \pm\frac{4e^2}{h}\left(N+\frac{1}{2}\right)\ (N \geq 0) \qquad \sigma_{xy} = \pm\frac{4e^2}{h}N\ (N \geq 1)$$

Bilayer graphene
: Massive chiral particles

Electric field



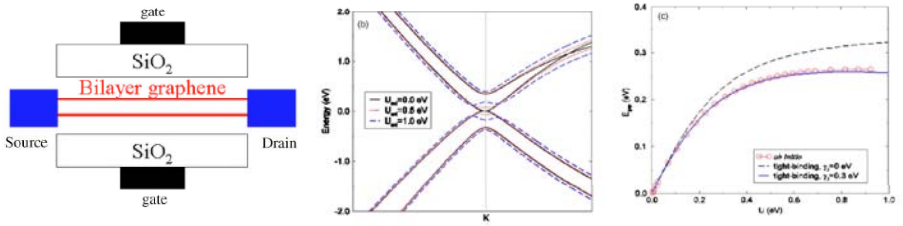
Δ

-Δ

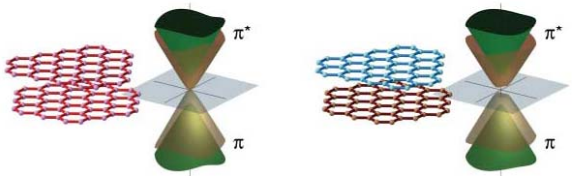
$$\mathcal{H}_{\text{eff}} \simeq \frac{v_F^2}{t_\perp}\begin{pmatrix} 0 & \pi^2 \\ (\pi^\dagger)^2 & 0 \end{pmatrix} \rightarrow H_{\text{eff}} \sim \begin{pmatrix} \Delta & \eta\pi^2 \\ \eta(\pi^\dagger)^2 & -\Delta \end{pmatrix} \qquad \eta = \frac{t_\perp^2 v_F^2}{\Delta^2 + t_\perp^2}$$

Transverse electric field can generate energy gaps in spectrum !!

Bilayer graphene
- Energy gap under perpendicular electric field



Min, McDonald *et al*, PRB **75**, 155115 (2007)
McCann, PRB **74**, 161403 (R) (2006)

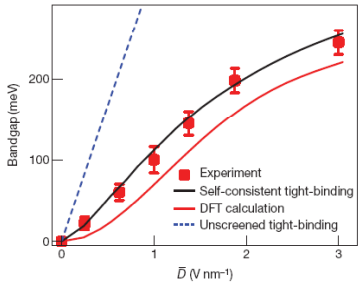


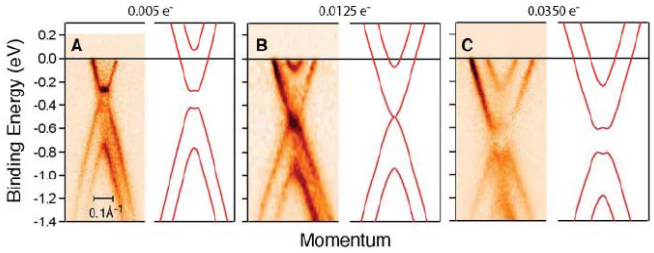
Bilayer graphene

- Energy gap under perpendicular electric field

Min, McDonald *et al*, PRB **75**, 155115 (2007)
McCann, PRB **74**, 161403 (R) (2006)

Oostinga *et al*, Nature Mat. **7**, 151 (2007)
Zhang *et al*, Nature **459**, 820 (2009)
T. Ohta *et al*, Science **313**, 951 (2006)





Lecture 3

Generalizations

Generalized Weyl Hamiltonian

- Relativistic invariance in two space dimensions

The most general Hamiltonian linear in the space **k**=(k_x,k_y)

$$\mathcal{H} = \sum_{\mu=0,\cdots 3} \mathbf{v}_\mu \cdot \mathbf{k}\sigma^\mu$$

$$\mathbf{v}_\mu = (v_\mu^x, v_\mu^y) \begin{cases} v_\mu^x = (v_0^x, \vec{v}^x) \equiv (v_0^x, v_1^x, v_2^x, v_3^x) \\ v_\mu^y = (v_0^y, \vec{v}_0^y) \equiv (v_0^y, v_1^y, v_2^y, v_3^y) \end{cases}$$

: 4 dimensional vectors in the SU(2) space

$$\sigma^\mu = (\sigma^0, \vec{\sigma}) \equiv (\mathbf{1}, \sigma^1, \sigma^2, \sigma^3)$$

$$\Rightarrow \quad \mathcal{H} = \mathbf{v}_0 \cdot \mathbf{k}\sigma^0 + (\vec{v}^x k_x + \vec{v}^y k_y) \cdot \vec{\sigma}$$

Generalized Weyl Hamiltonian

- Relativistic invariance in two space dimensions

$$\mathcal{H} = \mathbf{v}_0 \cdot \mathbf{k}\sigma^0 + (\vec{v}^x k_x + \vec{v}^y k_y) \cdot \vec{\sigma}$$

If $\mathbf{v}_0 = \mathbf{v}_4 = 0, \mathbf{v}_1 = (v_F, 0), \mathbf{v}_2 = (0, v_F)$

$$\mathcal{H} \to v_F(k_x\sigma^1 + k_y\sigma^2)$$: ideal graphene

If $\mathbf{v}_3 = 0$ and rotation of 2D frame,

$$\mathcal{H} \to \mathbf{w}_0 \cdot \mathbf{q}\sigma^0 + w_x q_x \sigma^x + w_y q_y \sigma^y$$

: Minimal Weyl Hamiltonian

M. O. Goerbig *et al*, PRB **78**, 045415 (2008)

Generalized Weyl Hamiltonian

- Relativistic invariance in two space dimensions

$$\mathcal{H} = \mathbf{w}_0 \cdot \mathbf{q}\sigma^0 + w_x q_x \sigma^x + w_y q_y \sigma^y$$

- Graphene Superlattices*
- Graphene under uniaxial strains**

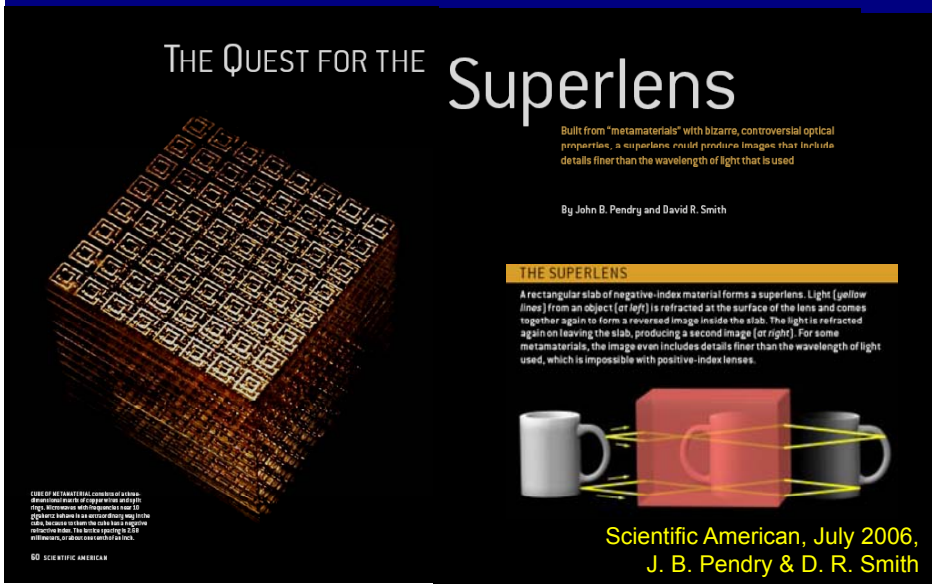
$$\mathcal{H} = m\sigma^z + w_x q_x \sigma^x + w_y q_y \sigma^y$$

- Epitaxial graphene***

* Park, **Son** *et al*, Phys. Rev. Lett. **101**, 126804 (08)
** Choi, Jhi, **Son**, *submitted* (09)
*** Kim, Ihm, Choi, **Son**, Phys. Rev. Lett. **100**, 176802 (08)
Kim, Ihm, Choi, **Son**, *submitted* (09)

Transport properties of graphene

- Superlattices: neutrino crystal ?

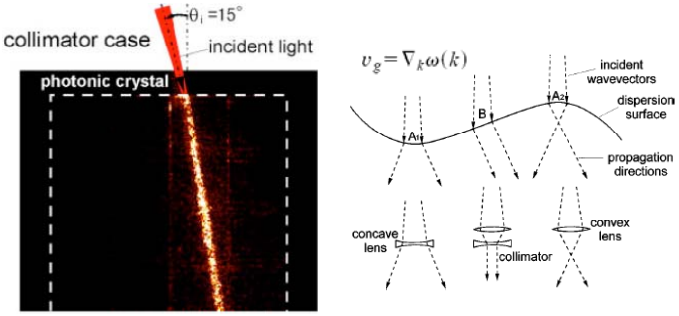


Scientific American, July 2006,
J. B. Pendry & D. R. Smith

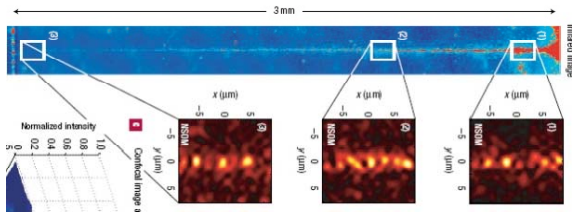
Graphene Superlattice

- Supercollimation in photonic crystals !

NEC
APL (99)

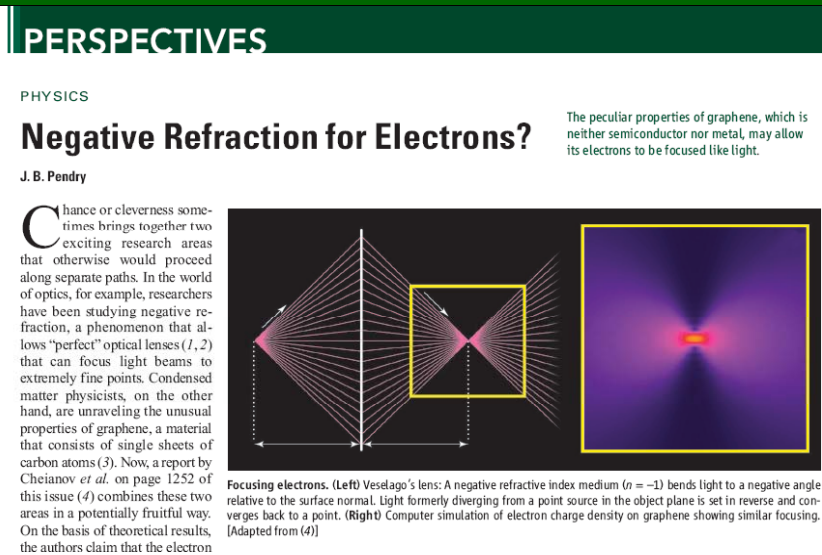


MIT
Nature Mat (06)



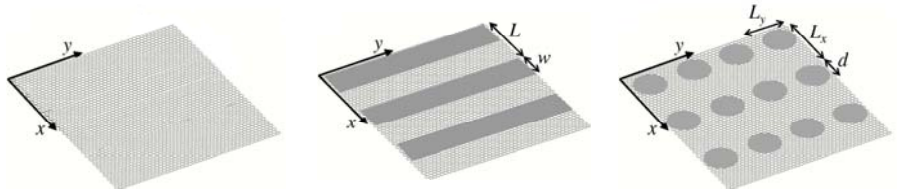
Graphene Superlattice

- Graphene superlens ?



Graphene Superlattice

- Neutrino crystal (?)



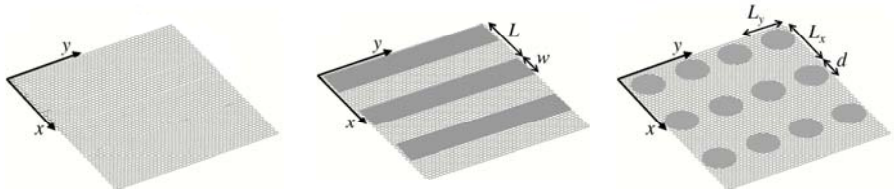
Pristine graphene | 1-D superlattice | 2-D superlattice

- Large scale (>>$d_{C\text{-}C}$) periodic potential imposed on pristine 2-D graphene
- Low energy effective Hamiltonian approach

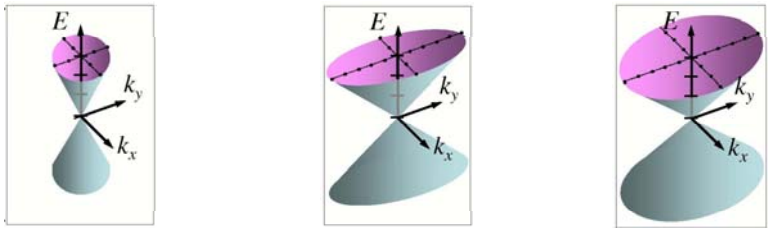
Park, Son, Louie *et al*, Nature Phys (08)

Graphene Superlattice

- Anisotropy from periodicity



Pristine graphene | 1-D superlattice | 2-D superlattice



Park, Yang, Son *et al*, Nature Phys (08)

Graphene Superlattice

- Equations

Scattering matrix: $\langle s, \mathbf{k} | U(\mathbf{r}) | s', \mathbf{k}' \rangle = \sum_{\mathbf{G}} \frac{1}{2} \left(1 + ss' e^{-i\theta_{\mathbf{k},\mathbf{k}-\mathbf{G}}}\right) U(\mathbf{G})\, \delta_{\mathbf{k}',\mathbf{k}-\mathbf{G}}$,

Central secular equation: ($\varepsilon_{s,\mathbf{k}} = s\hbar v_0 k$)

$$(E - \varepsilon_{s,k})\, c(s, \mathbf{k}) = \sum_{s',\mathbf{G}} \frac{1}{2} \left(1 + ss' e^{-i\theta_{\mathbf{k},\mathbf{k}-\mathbf{G}}}\right) U(\mathbf{G})\, c(s', \mathbf{k} - \mathbf{G})$$

G : reciprocal vector for superlattice potenital (<< K_+, K_-)

$e^{-i\theta}$: Angular dependent scattering matrix as a direct manifestation of chirality of electrons in graphene

Graphene Superlattice

- Equations

Scattering matrix: $\langle s, \mathbf{k} | U(\mathbf{r}) | s', \mathbf{k}' \rangle = \sum_{\mathbf{G}} \frac{1}{2} \left(1 + ss' e^{-i\theta_{\mathbf{k},\mathbf{k}-\mathbf{G}}}\right) U(\mathbf{G})\, \delta_{\mathbf{k}',\mathbf{k}-\mathbf{G}}$,

Central secular equation: ($\varepsilon_{s,\mathbf{k}} = s\hbar v_0 k$)

$$(E - \varepsilon_{s,k})\, c(s, \mathbf{k}) = \sum_{s',\mathbf{G}} \frac{1}{2} \left(1 + ss' e^{-i\theta_{\mathbf{k},\mathbf{k}-\mathbf{G}}}\right) U(\mathbf{G})\, c(s', \mathbf{k} - \mathbf{G})$$

1-D superlattice case with weak periodic potential :

$$\frac{v_{\hat{k}} - v_0}{v_0} = -\sum_{\mathbf{G}\neq\mathbf{0}} \frac{2|U(\mathbf{G})|^2}{v_0^2 |\mathbf{G}|^2} \sin^2 \theta_{\mathbf{k},\mathbf{G}}$$

1-D weak K-P potential case:

$$\frac{v_{\hat{k}} - v_0}{v_0} = -\left\{ \frac{U_{1D}^2 L^2}{\pi^4 v_0^2} \sum_{n>0} \frac{1}{n^4} \sin^2 \left(\frac{\pi w}{L} n\right) \right\} \sin^2 \theta_{\mathbf{k},\hat{x}}$$

Graphene Superlattice

- Anisotropy from periodicity (details)

Pristine graphene

$$H = \hbar v_F(\sigma_x p_x + \sigma_y p_y)$$

1-D superlattice

$$H = \hbar v_F(\sigma_x p_x + \sigma_y p_y + IV(x)/\hbar v_F)$$

$$H' = U_2^\dagger U_1^\dagger H U_1 U_2$$

$$\rightarrow H' = \hbar v_F(\sigma_x p_x + f_m \sigma_y p_y)$$

$$U_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-\frac{i\alpha(x)}{2}} & -e^{\frac{i\alpha(x)}{2}} \\ e^{-\frac{i\alpha(x)}{2}} & e^{\frac{i\alpha(x)}{2}} \end{pmatrix} \quad U_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

$$\alpha(x) = 2\int_0^x dx' V(x')/\hbar v_F$$

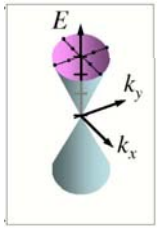
$$e^{-i\alpha(x)} = \sum_{m=-\infty}^{\infty} f_m[V] e^{imG_0 x}$$

Park, **Son** *et al*, PRL (08)

Transport properties of graphene

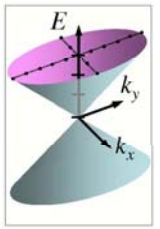
- Superlattices

Pristine graphene



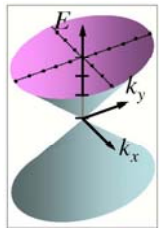
$$H = \hbar v_F(\sigma_x p_x + \sigma_y p_y)$$

1-D superlattice



$$H = \hbar(v_F \sigma_x p_x + v_{Fy} \sigma_y p_y)$$

2-D superlattice



$$H = \hbar(v_{Fx} \sigma_x p_x + v_{Fy} \sigma_y p_y)$$

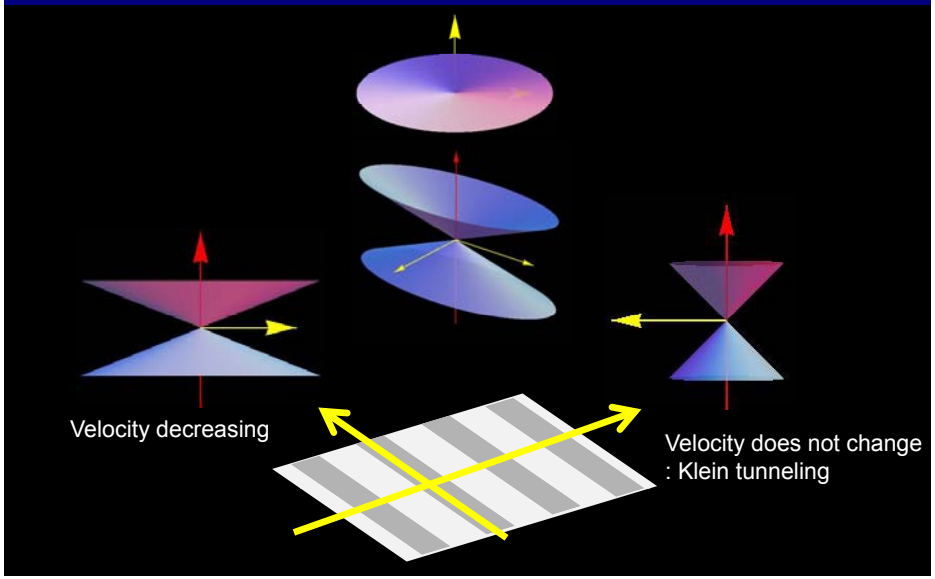
Dirac equation → Generalized Weyl's equation

Slowing down group velocity (eventually to zero)

Park, **Son** *et al*, Phys. Rev. Lett. (08,09), Nano Lett (08)

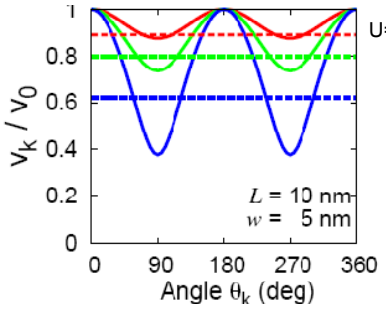
Transport properties of graphene

- Superlattices

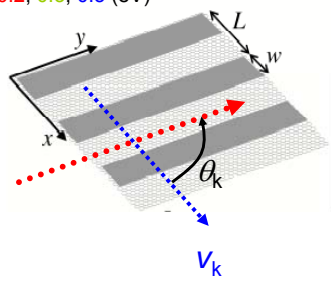


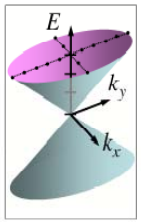
Graphene Superlattice

- Velocity renormalization under 1-D superlattice



U=0.2, 0.3, 0.5 (eV)



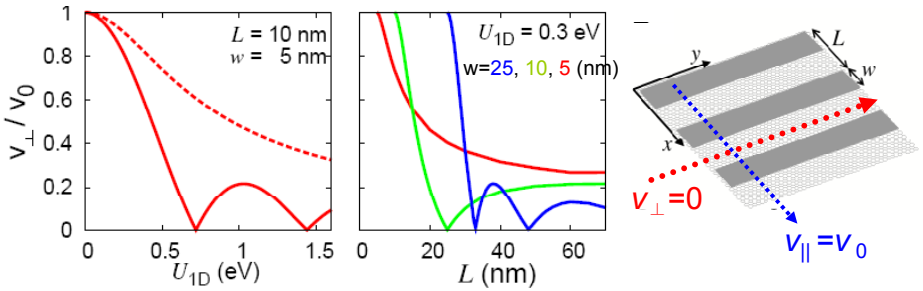


- Velocity across barrier is never reduced (Klein paradox)
- Velocity along barriers are strongly renormalized (reduced)
- Dirac cone is distorted to oblique shape in momentum space

Park, Son, Louie *et al*, Nature Phys (08)

Graphene Superlattice

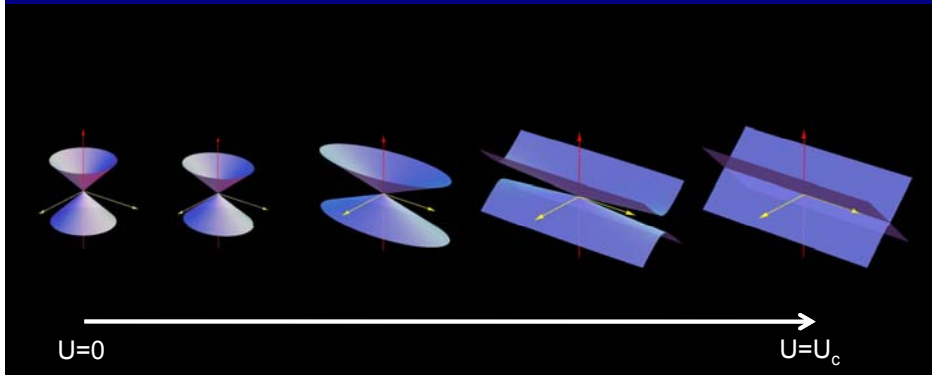
- Perfect zero velocity in one-direction



- For some critical U (or for some critical period L with fixed U), velocity along barriers is renormalized to zero
- Hence, we achieve one-dimensional graphene nanoribbons states without any cutting of sample

Transport properties of graphene

- Superlattices

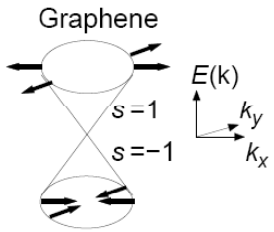


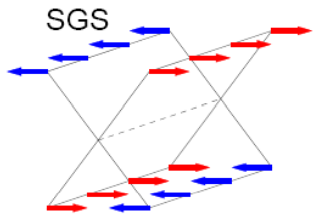
From isotropic Dirac cone to wedge shape one-dimensional dispersion !
(Direct consequence of chiral nature of carriers in graphene)

Park, **Son** *et al*, Nature Phys (08), PRL (08)

Graphene Superlattice

- Collapse of chirality or helicity





$$E_s^0(\mathbf{k}) = s\,\hbar\, v_0\,|\mathbf{k}|$$

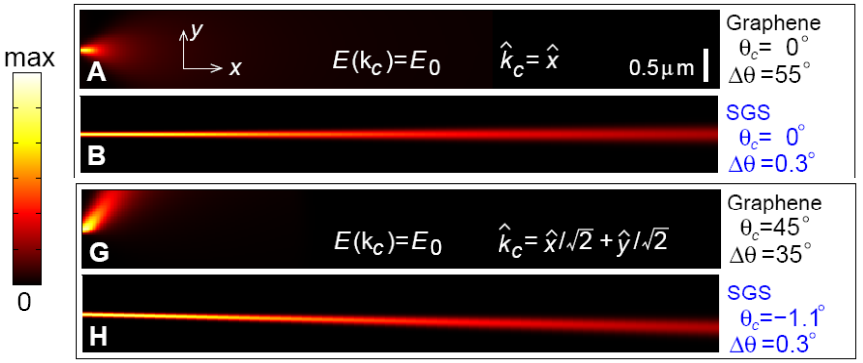
$$\psi^0_{s,\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ s\, e^{i\theta_\mathbf{k}} \end{pmatrix} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$E_s(\mathbf{k}) = s\hbar v_0 |k_x|$$

$$\psi_{s,\mathbf{k}}(\mathbf{r}) = e^{if(x)}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ s\ \mathrm{sgn}\ (k_x) \end{pmatrix} e^{i\mathbf{k}\cdot\mathbf{r}}$$

Graphene Superlattice

- Prediction of electron supercollimation

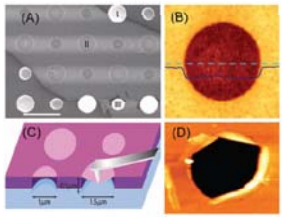


$$E(\mathbf{k}_c) = E_0 = \hbar v_0\, 0.1\pi/L = 0.02\ \mathrm{eV}$$

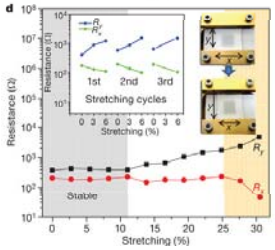
- One directional propagation of electron wave packet with negligible spatial spreading (0.1 mm propagation with 500 nm spreading)
- Analogue to quantum Hall edge state ?
- Possible quantum interferometry

Strained graphene

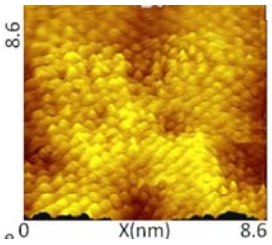
Graphene is the strongest material ever measured &
the thinnest membrane ever created



J. Hone, Science (2008)



B. Hong, Nature (2009)

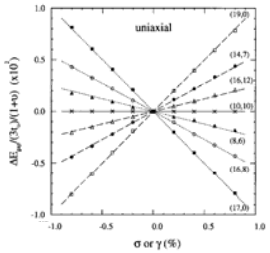


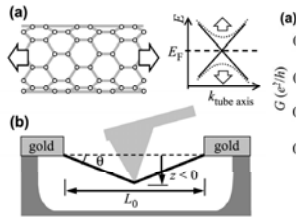
N.-C. Yeh, Nano Lett (2009)

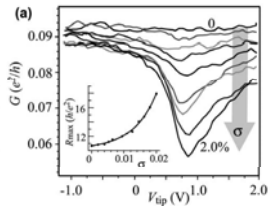
• Strains can be applied intentionally or naturally

Strained graphene

- Previous lessons from carbon nanotubes





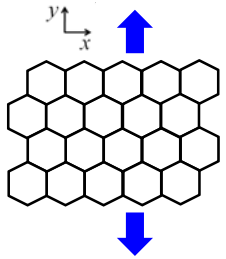


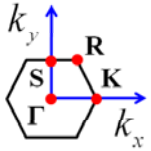
L. Yang & J. Han, PRL **85**, 154 (00) E. D. Minot *et al*, PRL **90**, 156401 (03)

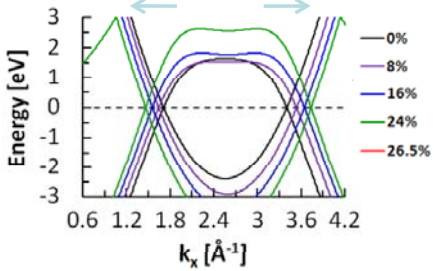
Strained carbon nanotubes: Metal-to-Semiconductor or
Semiconductor-to-Metal transition depending on chiralities

Strained graphene

- Electronic structures with strains from first-principles



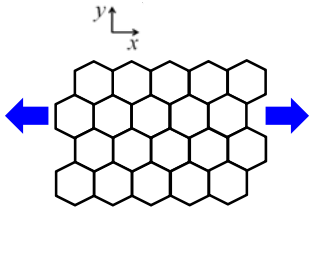


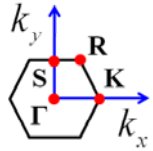


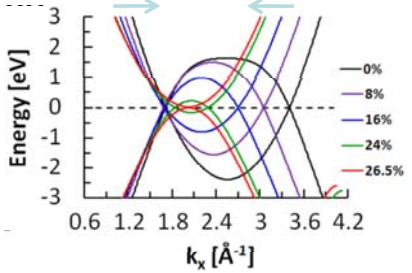
- Strain along armchair direction (A-strain)
- No bandgap opening up to 26.5% strain
- Repulsion between K and K' points

Strained graphene

- Electronic structures with strains from first-principles

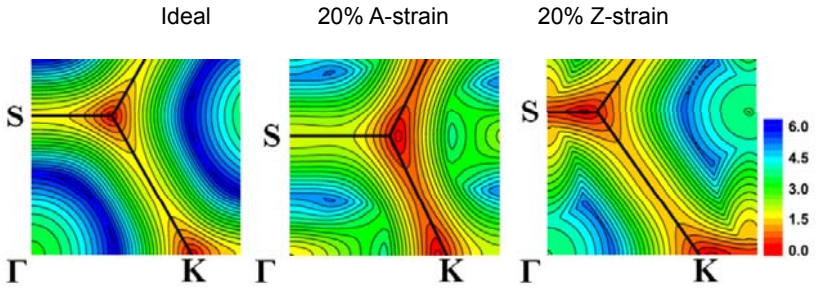






- Strain along zigzag direction (Z-strain)
- No bandgap opening up to 26.5% strain
- Merging two K points

Strained graphene
- Energy contours

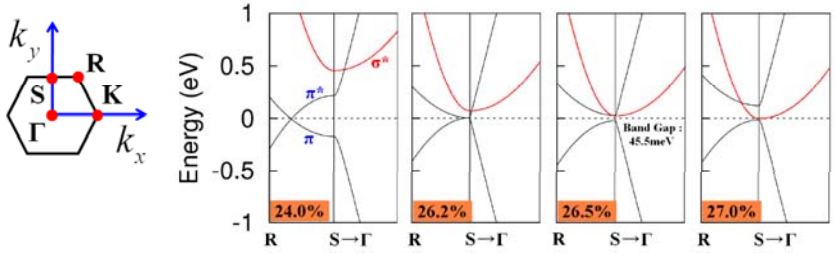


- Mismatch between Dirac points and high symmetric points in Brillouine zone (strain as vector potential*)

$$H = v_F \vec{\sigma} \cdot \vec{p} \longrightarrow H = v_F \vec{\sigma} \cdot (\vec{p} - \vec{A})$$

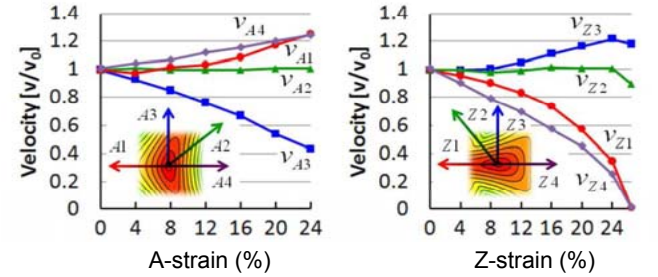
* A. H. Castro Neto *et al*, RMP (09)
F. Guinea *et al*, Nature Phys (09)

Strained graphene
- Large magnitude of Z-strain



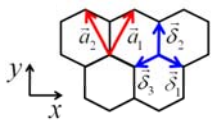
- Merging of Dirac points induce energy gaps with Z-strains
- Shiftdown of σ*-bands toward to Fermi energy
- Very narrow window for gap in very high strains
- Coexistence of massive and massless electrons

Strained graphene
- Anisotropy in group velocity at Dirac point



- *Increase* of velocity in direction perpendicular to strains : improvement of mobility?
- Quick decrease of velocity in direction parallel to strains
- $v_{A1} \neq v_{A4}$
- $v_{Z1} \neq v_{Z4}$

Strained graphene
- Effective Hamiltonian 1



$$\mathcal{H} = -t_2 \sum_k \left[\xi(k) c^\dagger_{Ak} c_{Bk} + c.c. \right]$$

$$t_i \equiv t(\delta_i) \quad \xi(k) = e^{k \cdot \delta_2} (1 + 2\eta e^{-ik_y a_y} \cos(k_x a_x))$$

$$\eta \equiv t_1/t_2 = t_3/t_2 \quad \text{<1 (>1) for Z (A) strain}$$

Expanding $\xi(k)$ around $k_D = \frac{1}{a_x} \cos^{-1}(-\frac{1}{2\eta})$

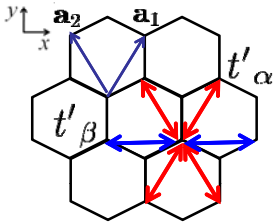
$$\xi(\mathbf{q}) = \xi(k_D + q_x, q_y) \simeq (4\eta^2 - 1)^{1/2} a_x q_x - i a_y q_y$$

$$v_x = t_2 a_x (4\eta^2 - 1)^{1/2}, v_y = t_2 a_y$$

$$\longrightarrow \boxed{\mathcal{H} \simeq v_x \sigma_x q_x + v_y \sigma_y q_y}$$

Not sufficient for description of the results from first-principles calculations

Strained graphene
- Effective Hamiltonian 2



Next nearest neighbor hopping t'

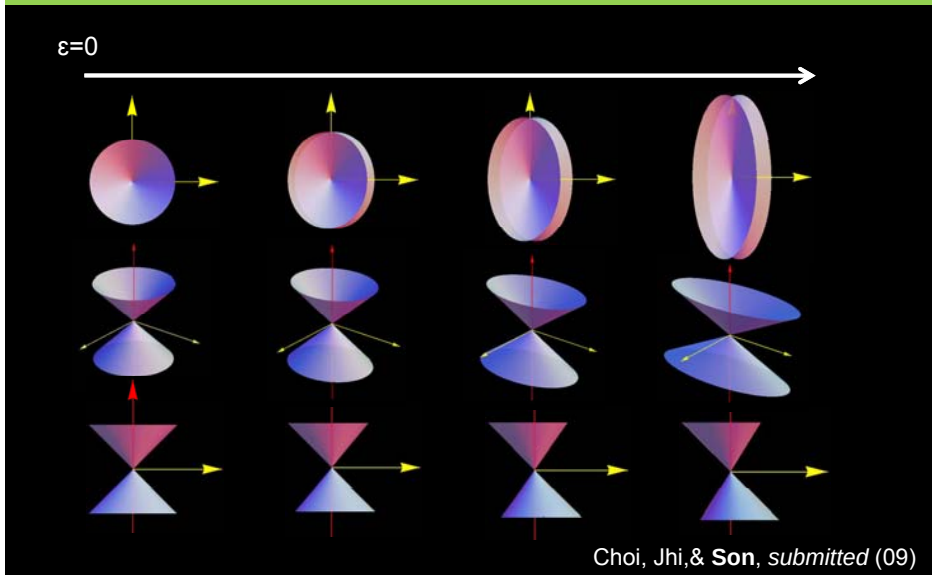
: quadratic (q^2) order in ideal graphene but *linear* (q) in strained graphene

$$t'_\alpha \equiv t'(\pm\mathbf{a}_1) = t'(\pm\mathbf{a}_2),$$
$$t'_\beta \equiv t'(\pm(\mathbf{a}_1 - \mathbf{a}_2)),$$
$$\chi \equiv t'_\beta/t'_\alpha < 1 (> 1) \quad \text{for Z (A) strain}$$

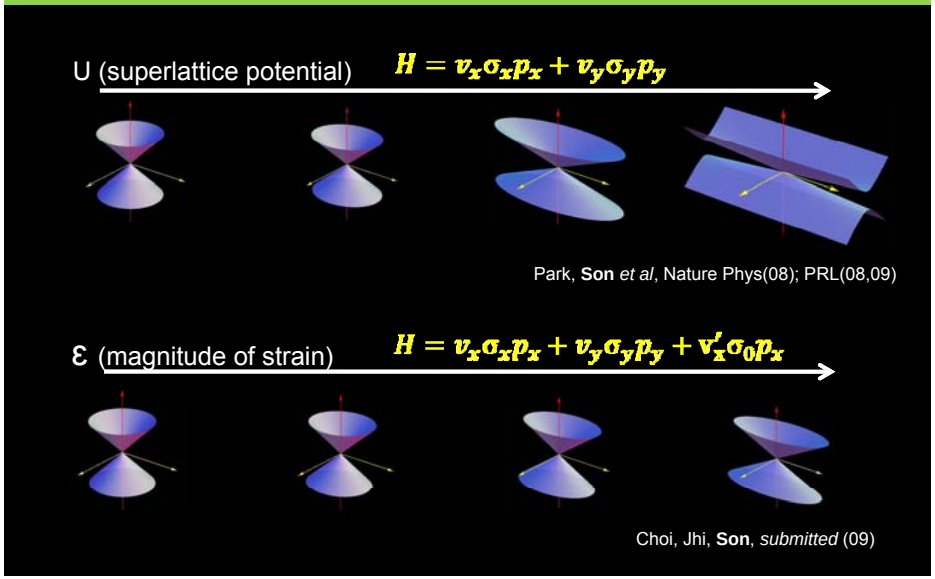
$$\mathcal{H}' \simeq v'_x q_x \sigma_0$$

$$(v'_x = a_x t'_\alpha (1-\chi/\eta)(4-1/\eta^2)^{1/2})$$

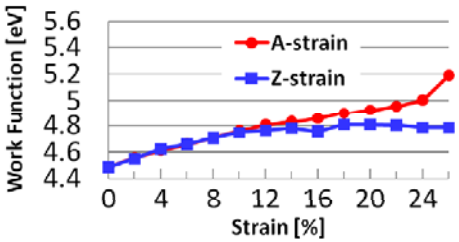
Strained graphene
- Tilted anisotropic Dirac cones



Generalized Weyl Hamiltonian
- Superlattice vs. Strains

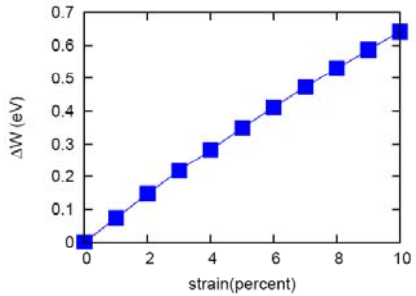


Strained graphene
- Work functions



- Increasing work function as increasing *uniaxial homogeneous strain* (strain as scalar potential)
- With very large strain, work function differs depending on the direction of strains
- Controlled charge transfer between impurities (metal) and graphene by strain ?

Strained graphene
- Work functions



- *Isotropic* strain : (almost) linear increase of work function
- Strain is equivalent to effective 'scalar potential'

Choi, Jhi, Son, *submitted*

Strained graphene
- Effective Hamiltonian

Effective Hamiltonian for ideal graphene

$$H = v_F(\sigma_1 p_1 + \sigma_2 p_2)$$

↓

Effective Hamiltonian for strained graphene

$$H = \sum_{\alpha=0,1,2} v_\alpha \sigma_\alpha (p_\alpha - A_\alpha) + \phi_{st}$$

No energy gap for any homogeneous strains