Relativistic Dirac Electrons in Solids

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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)

What is graphene?
- Carbon allotropes

Lecture 1

Relativistic Dirac Electrons in Graphene
**Why Carbon?**

This slide 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 exotic at RT

**Graphene**

- Statistics of recent APS March meetings

2009 APS March meeting at Pittsburg, USA

**DCMP**: Graphene Focus Sessions I-XIX
(Organizers: 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?)
Brief history of graphene

- Early works

  • Intercalated graphite as a route to graphene

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

- Isolation of graphene

  • Micromechanical cleavage of bulk graphite up to 100 μm in size via adhesive tapes

Electronic structure of graphene

- 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 92037
  (Received 16 September 1981)

  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.

- Isolation of graphene

  • Micromechanical cleavage of bulk graphite up to 100 μm in size via adhesive tapes

- Breakthrough

  • Micromechanical cleavage of bulk graphite up to 100 μm in size via adhesive tapes
**Epitaxial Graphene**
- Graphene electronics?

- Epitaxial growth of graphene on SiC{0001}
  
  W. A. de Heer Group at Georgia Tech  

- 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  

  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

- $sp^2$ bonding
- $sp^3$ bonding

Hexagonal network of Carbon

- $sp^2$ bonding

**Electronic structure of graphene**
- Real space: tight-binding Hamiltonian

- Two sublattices - Bipartite system

- Nearest-neighbor tight-binding Hamiltonian for $\pi$-orbitals

$$\mathcal{H} = -t \sum_{r \in A} \sum_{i=1,2,3} \left[ a_i^\dagger(r) b(r + s_i) + b_i^\dagger(r + s_i) a(r) \right]$$
Electronic structure of graphene
- Energy spectrum

\[ H = \sum_{k} \left[ \Phi(k) a_{\uparrow}(k) b_{\downarrow}(k) + \Phi^{*}(k) a_{\downarrow}(k) b_{\uparrow}(k) \right] \]

\[ E(k) = + \varepsilon(k) = + \left| 1 + 2a_{\gamma} e^{i\gamma(k)} \cos \left( \frac{\sqrt{3} k_x}{2a} \right) \right| \]

- Hexagonal BZ with two special Fermi points,

\[ K_{\pm} = \left( \pm \frac{4\pi}{3\sqrt{3}a}, 0 \right) \]

Electronic structure of graphene
- Linear energy bands

- Two inequivalent Dirac cones at \( K \) and \( K' \)

\[ \Phi_{\pm}(p) = t \sum_{j=1,2,3} e^{-i(K_{\pm} + p) \cdot s_j} \]

\[ \cong t \sum_{i=1,2,3} e^{-iK_{\pm} \cdot s_j} \left( i p \cdot s_i \right) \]

\[ = \frac{3\pi}{2} \left( p_x - i p_y \right) = v_F \left( p_x - i p_y \right) \]

Electronic structure of graphene
- Real space

Two sublattices - Bipartite system

\[ \text{Spin Up} \quad \text{(Pseudo)} \quad \text{Spin Down} \quad \text{(Pseudo)} \]

Electronic structure of graphene
- ‘Neutrino’ in your pencil?

\[ H = v_F \left( \sigma_x p_x + \sigma_y p_y \right) = v_F \sigma \cdot p \]

Dirac equation with zero mass

charged ‘neutrino’ in your pencil?

- Relativistic particle :

\[ E = \pm \sqrt{c^2 p^2 - m^2 c^4} = \pm v_F |p| \]

\( c = v_F \): effective speed of ‘light’

\( m = 0 \)
**Electronic structure of graphene**
- Consequences of massless Dirac fermions

**Linear Density of States**

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

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

Zhang et al., Novoselov et al (05)

**Transport properties of graphene**
- Mobility of graphene

Mobility of suspended graphene $\sim 200,000$ cm$^2$/Vs

Observation of nearly ballistic transport regime/ FQHE


**Electronic structure of graphene**
- Total Hamiltonian

$$H_{\text{tot}}(p) = v_F [p_x (\sigma \otimes \tau_z) + p_y (\sigma \otimes 1_2)]$$
with \(\psi = \begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix}\)

\(\sigma\) acts on sublattice A (B) and \(\tau\) on $K_+$ ($K$)

**Electronic structure of graphene**
- Gap generation in graphene

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

Onsite energy difference - Mixing pseudo-spins

Mixing between $K_+$ and $K$
- Mixing chiralities

$$H = \begin{pmatrix} KA & KB \\ KB^* & K'B \end{pmatrix}$$

$$KA = v_F (\hat{k}_x - i\hat{k}_y)$$

$$KB = v_F (\hat{k}_x + i\hat{k}_y)$$

$$K'B = v_F (\hat{k}_x + i\hat{k}_y)$$

$$K'A = 0$$

$$|2\alpha|$$

$$|2\beta|$$
Electronic structure of graphene

- Low energy dispersions

\[ H = v_F (\sigma_x p_x + \sigma_y p_y) = v_F \sigma \cdot p \]

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

- Pseudospin and chiral states

\[ H - v_F (\sigma_x p_x + \sigma_y p_y) - v_F \sigma \cdot p \]

Eigenfunctions: Spinor representation

\[ \psi_c = e^{-i \frac{\theta_p}{2}} |1\rangle + e^{i \frac{\theta_p}{2}} |0\rangle \]

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

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

- Chiral states: charged "neutrino" in your pencil

Helicity operator: \( \hat{h} = \frac{1}{2} \sigma \cdot \hat{p} \)

- Conduction band:

\[ \hat{h} \psi_c = \frac{1}{2} \sigma \cdot \hat{p} \psi_c = \frac{1}{2} \psi_c \]

\( \sigma_x = -1/2 \quad \to \quad \sigma_x = +1/2 \)

\( p_x < 0 \quad \to \quad p_x > 0 \)

- Consequence of chirality

- Eigenstates:

\[ \langle r | \sigma_p + \rangle = \psi_{\sigma_p +}(r) = \frac{1}{\sqrt{2}} e^{ip \cdot \tau} R^{-1}(\theta_p) \left( \frac{1}{\epsilon} \right) \]

- For a long-range disorder where \( |q| \ll K \) a elastic scattering matrix element is

\[ |\langle \sigma_p' | V | \sigma_p \rangle|^2 = |V(p' - p)|^2 \cos^2 \left( \frac{\theta_p - \theta_{p'}}{2} \right) \]

: Complete absence of backscattering (pseudospin conservation)


**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.

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**Lecture 2**
Consequences

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**Electronic structure of graphene**
- Tunneling

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**Electronic structure of graphene**
- Klein paradox

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

- Klein paradox: Unimpeded penetration of relativistic particles through very high potential barriers.
- Potential drop \( \sim 2mc^2 \) over \( \frac{h}{mc} \approx 10^8 \) V/Å
  - Event horizon of Black hole
  - Supercritical massive atoms

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Electronic structure of graphene

- **Klein tunneling**

- **Klein tunneling**


  V. V. Cheianov *et al.*, Science **315**, 1252 (2007)


**Transport properties of graphene**

- **Klein tunneling**

**Electronic structure of graphene**

- **Klein tunneling**

  Pabry-Ferot interference: observation of Berry's phase


**Electronic structure of graphene**

- **Klein paradox**

  *Supercritical atomic collapse if Z ≥ 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

\[ \psi(p) = R^{-1}(\theta_p) \begin{pmatrix} 1 \\ i \end{pmatrix} \]
\[ R(\theta_p) = \exp \left( \frac{\theta_p}{2} \sigma_z \right) \begin{pmatrix} e^{i\theta_p} & 0 \\ 0 & e^{-i\theta_p} \end{pmatrix} \]
\[ R(\theta_p \pm 2\pi) = -R(\theta_p) \]
\[ \Delta R_{xx} = -R(B, T) \cos \left( \frac{2\pi B}{B_p} + 2\pi \phi \right) \]

Landau orbit near Fermi level

Electronic structure of graphene
- Landau levels in perpendicular B-field

Parabolic band (normal metal)
\[ E_n = \frac{\hbar c}{2m} \left( n + \frac{1}{2} \right) \]
\[ \omega_c = \frac{eB}{mc} \]
\[ l_p = \frac{\hbar c}{eB} \]
\[ B = 10 T, \quad \hbar \omega_c = 1 K \]

Linear band (single layer graphene)
\[ E_n = \frac{\hbar c \sqrt{n}}{2} \]
\[ \omega_c = \frac{v_F}{l_p} = \frac{eB}{\hbar c} \]
\[ B = 10 T, \quad \hbar \omega_c \approx 1500 K \]

Electronic structure of graphene
- Consequences of chiral massless Dirac fermions

Half-integer Quantum Hall Effect (Room T)!
(Manifestation of Berry’s phase of pseudospin)

\[ R_{xy} = \pm g_s \cdot \left( \frac{\theta}{2} + \frac{1}{2} \right) \cdot \frac{e^2}{h} \]
\[ n = 1, 2, 3, \ldots \]
\[ g_s = 2 \times 2 \ (\text{spin} \ & \text{sublattice}) \]

Zhang et al (05), Novoselov et al (05)
Kim & Geim et al (07)
Haldane (88), T. Ando (02)

Electronic structure of graphene
- Consequence of chiral massless Dirac particles

Photoemission experiments:
Crescent shape anisotropy
(a 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


Electronic structure of graphene
- Gap?

Fine structure constant, \( \alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137} \)

“Effective Fine structure constant” in graphene:
\[ \alpha_G = \frac{e^2}{\hbar v_F} \approx \frac{300}{137 \times \epsilon} \]

PRL 102, 026802 (2009)

Electronic structure of graphene
- Opacity

Fine Structure Constant Defines Visual Transparency of Graphene


Transmittance ~ 97.7%
Electronic structure of graphene
- Opacity

<table>
<thead>
<tr>
<th>Material</th>
<th>Transparence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poly-PMO</td>
<td>0.02%</td>
</tr>
<tr>
<td>ITO</td>
<td>6.5% ± 1.1%</td>
</tr>
<tr>
<td>Air</td>
<td>6.46%</td>
</tr>
</tbody>
</table>

- Transparent flexible display?
- Replacement of ITO?
- Prof. Byung Hee Hong
  (SKKU) arXiv.org:0912.5485

See Video >>>

Bilayer Graphene

What is bilayer graphene?

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

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

\[ H = \begin{pmatrix} 0 & u_F & 0 & 0 \\ u_F & 0 & t_{\perp} & 0 \\ 0 & t_{\perp} & 0 & u_F \\ 0 & 0 & u_F & 0 \end{pmatrix} \]

\[ \Psi = (\psi_{B_1}, \psi_{A_1}, \psi_{B_2}, \psi_{A_2})^T \]
Bilayer graphene: Massive chiral particles

**Bilayer Graphene**

Low energy effective Hamiltonian by integrating out high energy dimer part

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

\[ m^* = \frac{t_\perp}{2v_F}, \quad \hat{n}_p = (\cos(2\theta_p), \sin(2\theta_p)) \]

**Single layer Graphene**

\[ \mathcal{H}_{\text{eff}} \simeq v_F \begin{pmatrix} 0 & \pi \\ \pi^\perp & 0 \end{pmatrix} = v_F |p| \sigma \cdot \hat{n}_p \]

\[ \hat{n}_p = (\cos(2\theta_p), \sin(2\theta_p)) \]

Transverse electric field can generate energy gaps in spectrum!!

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)


Generalized Weyl Hamiltonian
- Relativistic invariance in two space dimensions

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

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

$$v_\mu = (v_\mu^x, v_\mu^y) \begin{cases} v_\mu^x = (v_0^x, \bar{v}_x, v_1^x, v_2^x, v_3^x) \\ v_\mu^y = (v_0^y, \bar{v}_y, v_1^y, v_2^y, v_3^y) \end{cases}$$

$\sigma^\mu = (\sigma^0, \sigma^1, \sigma^2, \sigma^3)$

$$\mathcal{H} = v_0 \cdot k \sigma^0 + (\bar{v}^x k_x + \bar{v}^y k_y) \cdot \vec{\sigma}$$

Lecture 3
Generalizations

Generalized Weyl Hamiltonian
- Relativistic invariance in two space dimensions

$$\mathcal{H} = v_0 \cdot k \sigma^0 + (\bar{v}^x k_x + \bar{v}^y k_y) \cdot \vec{\sigma}$$

If $v_0 = v_4 = 0, v_1 = (v_F, 0), v_2 = (0, v_F)$

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

If $v_3 = 0$ and rotation of 2D frame,

$$\mathcal{H} \rightarrow w_0 \cdot q \sigma^0 + w_x q_x \sigma^x + w_y q_y \sigma^y$$

$\sigma^\mu = (\sigma^0, \sigma^1, \sigma^2, \sigma^3)$

: Minimal Weyl Hamiltonian

M. O. Goerbig et al, PRB 78, 045415 (2008)
Generalized Weyl Hamiltonian
- Relativistic invariance in two space dimensions

\[ \mathcal{H} = w_0 \cdot q^0 + w_x q_x \sigma^x + w_y q_y \sigma^y \]

- Graphene Superlattices*
- Graphene under uniaxial strains**

\[ \mathcal{H} = m \sigma^2 + w_x q_x \sigma^x + w_y q_y \sigma^y \]
- 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?

Graphene Superlattice
- Supercollimation in photonic crystals!

NEC APL (99)

MIT Nature Mat (06)

Graphene Superlattice
- Graphene superlens?

NEC AP L (99)

MIT Nature Mat (06)

Negative Refraction for Electrons?

The peculiar properties of graphene, which is a two-dimensional material made of carbon atoms, allow its electrons to be focused like light.
Graphene Superlattice

- Neutrino crystal (?)

  - Large scale (>>d_{C-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

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

Graphene Superlattice

- Equations

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

Central secular equation: \( (E - \varepsilon_{s,k}) c(s, k) = \sum_{s'G} \frac{1}{2} \left( 1 + s s' e^{-i\theta_{k,k'-G}} \right) U(G) c(s', k - G) \)

\( G \): reciprocal vector for superlattice potential \((<< K_s, K_p)\)

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

1-D superlattice case with weak periodic potential:

\[
\frac{v_k - v_0}{v_0} = -\sum_{G \neq 0} \frac{2 |U(G)|^2}{v_0^2 |G|^2} \sin^2 \theta_{k,G} \]

1-D weak K-P potential case:

\[
\frac{v_k - v_0}{v_0} = -\left( \frac{U_0^2 L^2}{\pi^2 v_0} \sum_{n \neq 0} \frac{1}{n^4} \sin^2 \left( \frac{\pi n L}{L} \right) \right) \sin^2 \theta_{k,i} \]
Graphene Superlattice
- Anisotropy from periodicity (details)

Pristine graphene

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

1-D superlattice

\[ H' = U_1^2 U_2^2 H U_1 U_2 \]

\[ H' = \hbar v_F (\sigma_x p_x + \sum f_m \sigma_y p_y) \]

\[ U_1 = \frac{1}{\sqrt{2}} \left( \begin{array}{cc} e^{-i\alpha(x)/2} & 0 \\ 0 & e^{i\alpha(x)/2} \end{array} \right) \]

\[ U_2 = \frac{1}{\sqrt{2}} \left( \begin{array}{cc} 1 & 1 \\ -1 & 1 \end{array} \right) \]

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

\[ e^{-i\alpha(x)} = \sum_{m=-\infty}^{\infty} f_m [V]\delta^{im}\zeta_{QX} \]

Park, Son et al, PRL (08)

Transport properties of graphene
- Superlattices

Pristine graphene

1-D superlattice

2-D superlattice

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

\[ H = \hbar v_F (\sigma_x p_x + \sum f_m \sigma_y p_y) \]

Dirac equation

\[ \text{Generalized Weyl's equation} \]

Slowing down group velocity (eventually to zero)

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

Transport properties of graphene
- Superlattices

- Velocity renormalization under 1-D superlattice

Velocity decreasing

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

\[ U=0.2, 0.3, 0.5 \text{ (eV)} \]

\[ v_k / v_0 \]

\[ L = 12 \text{ nm}, w = 5 \text{ nm} \]

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

Graphene Superlattice
- Prediction of electron supercollimation

- 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

- Previous lessons from carbon nanotubes

- Electronic structures with strains from first-principles

• Strains can be applied intentionally or naturally

J. Hone, Science (2008)  
B. Hong, Nature (2009)  
N.-C. Yeh, Nano Lett (2009)

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

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

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

- Ideal 20% A-strain 20% Z-strain

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

\[ H = v_F \vec{p} \rightarrow H = v_F \vec{p} \cdot (\vec{p} - A) \]


Strained graphene
- Large magnitude of Z-strain

• Merging of Dirac points induce energy gaps with Z-strains
• Shiftdown of \( \sigma^* \)-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

\[ H = -t_2 \sum_k [\xi(k) c_{Ak} c_{Bk} + c.c.] \]

\[ t_1 \equiv t(\delta_1) \quad \xi(k) = e^{i k_x (1 + 2v_F^{-1} k_y a_y \cos(k_y a_y))} \]

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

Expanding \( \xi(k) \) around \( k_D = \frac{1}{a_x} \cos^{-1}\left(-\frac{1}{a_x}\right) \)

\[ \xi(\eta) = \xi(k_D + q_x, q_y) \sim (4\eta^2 - 1)^{1/2} \alpha_x q_x - i n_y q_y \]

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

\[ H \approx \eta x \sigma_x \sigma_x \sigma_x + v_y \sigma_y \sigma_y \]

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

\[ t'_\alpha = t' (\pm a_1) - t' (\pm a_2), \]
\[ t'_\beta = t' (\pm (a_1 - a_2)), \]
\[ \chi \equiv t'_\beta / t'_\alpha < 1 (> 1) \text{ for } Z (A) \text{ strain} \]

\[ \mathcal{H}' \simeq v'_x q_x \sigma_0 \]

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

Strained graphene
- Tilted anisotropic Dirac cones

\[ \varepsilon = 0 \]

Choi, Jhi, & Son, submitted (09)

Generalized Weyl Hamiltonian
- Superlattice vs. Strains

\[ H = v_x \sigma_x p_x + v_y \sigma_y p_y \]

Park, Son et al, Nature Phys(08); PRL(08,09)

\[ H = v_x \sigma_x p_x + v_y \sigma_y p_y + v'_z \sigma_0 p_z \]

Choi, Jhi, Son, submitted (09)

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

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Strained graphene
- Effective Hamiltonian

Effective Hamiltonian for ideal graphene

\[ H = \nu_F (\sigma_1 p_1 + \sigma_2 p_2) \]

Effective Hamiltonian for strained graphene

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

*No* energy gap for any homogeneous strains