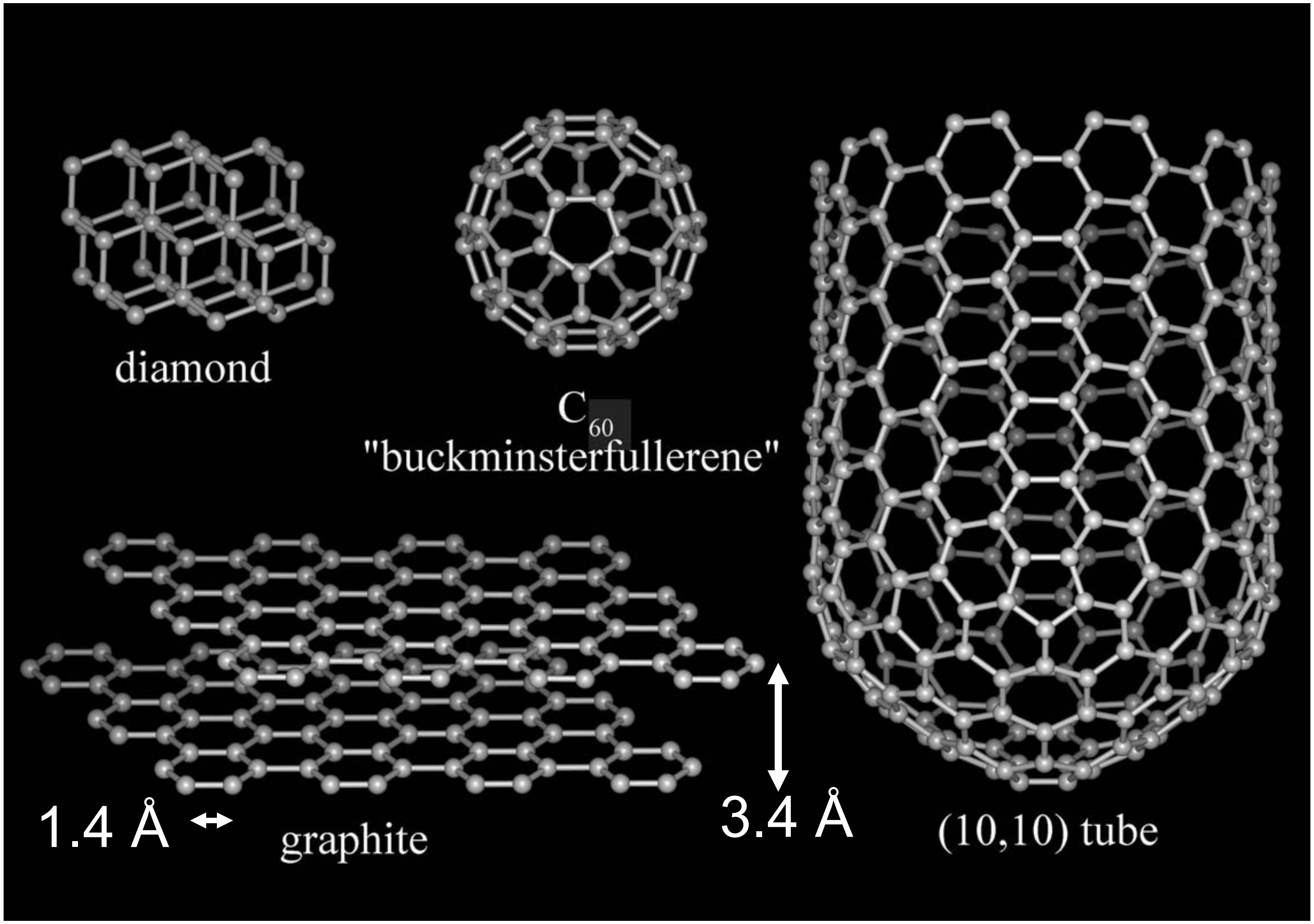
Quantum Theory of Graphene

- Graphene's electronic structure:
  A quantum critical point
- Emergent relativistic quantum mechanics:
  The Dirac Equation
- Insights about graphene from relativistic QM
  Insights about relativistic QM from graphene
- Quantum Hall effect in graphene

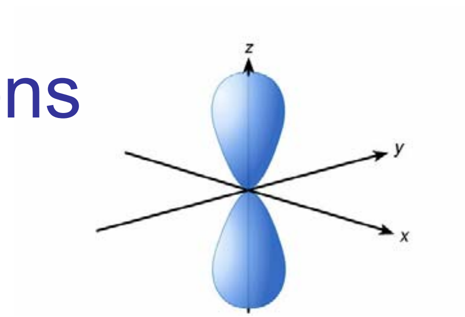
Allotropes of elemental carbon

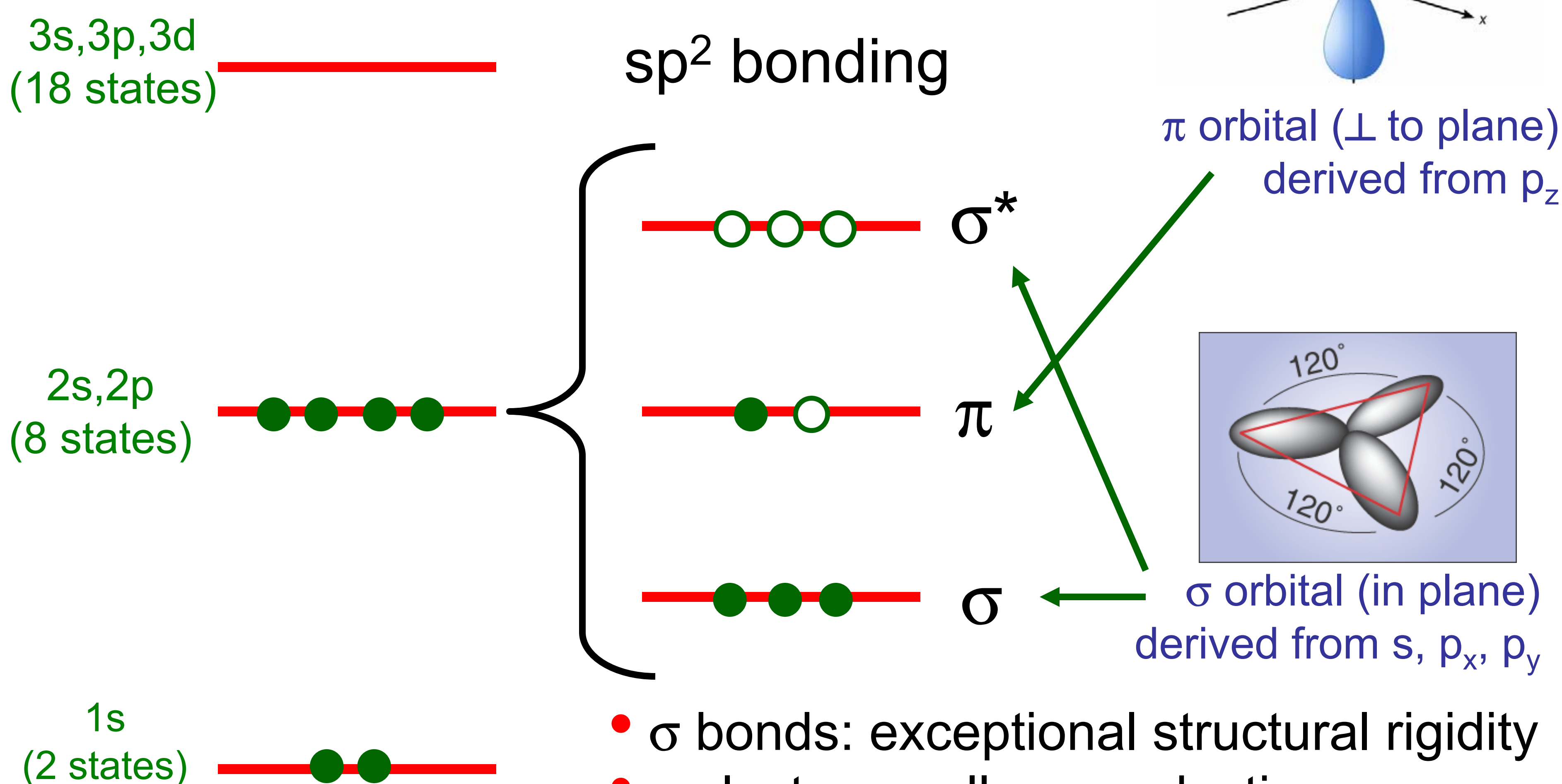


Graphene = A single layer of graphite

Graphene Electronic Structure

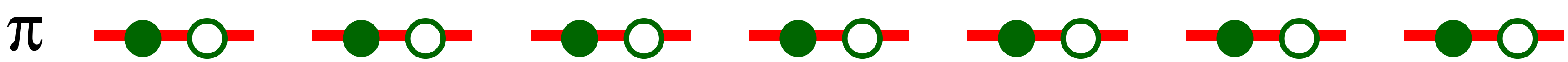
Carbon: Z=6 ; 4 valence electrons



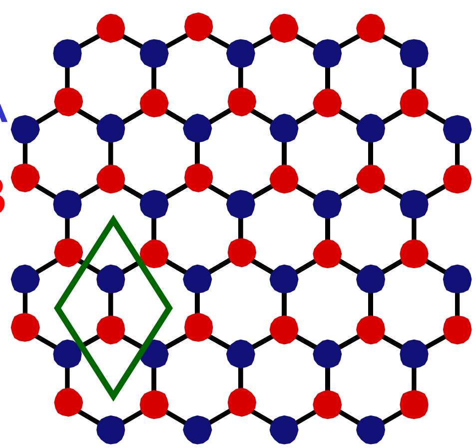


- σ bonds: exceptional structural rigidity
- π electrons: allow conduction

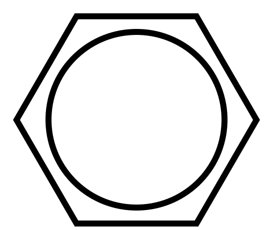
Hopping on the Honeycomb



Textbook QM problem: Tight binding model on the Honeycomb lattice

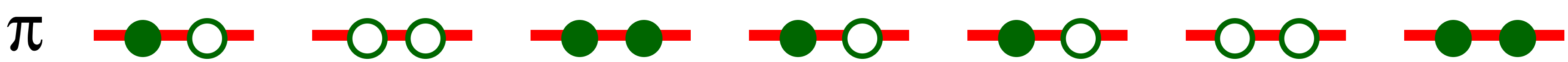


Just like CJ's homework!



Benzene
C_6H_6

Hopping on the Honeycomb



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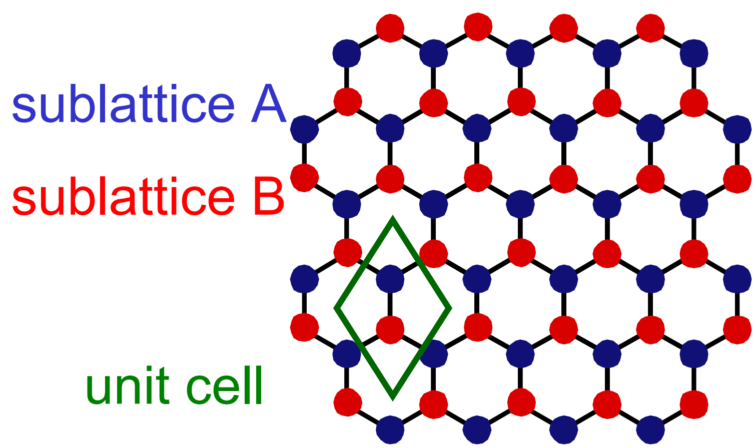

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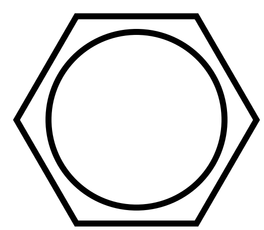
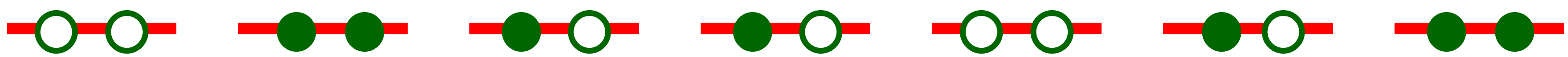


Benzene
C_6H_6

Hopping on the Honeycomb

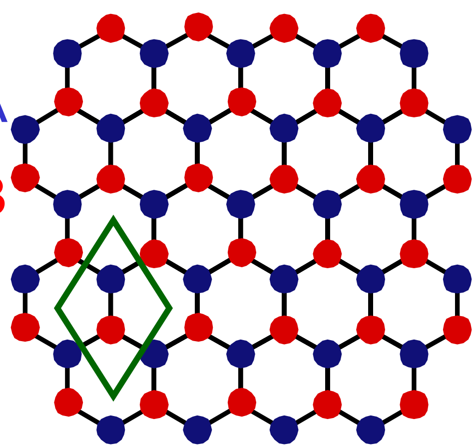
π 

Textbook QM problem: Tight binding model on the Honeycomb lattice

sublattice A

sublattice B

unit cell



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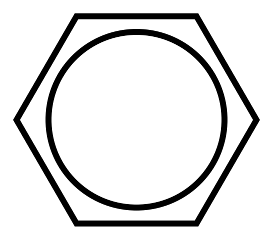


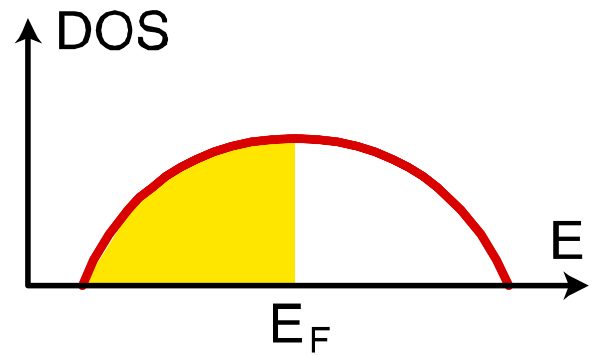
Benzene

C_6H_6

Electronic Structure

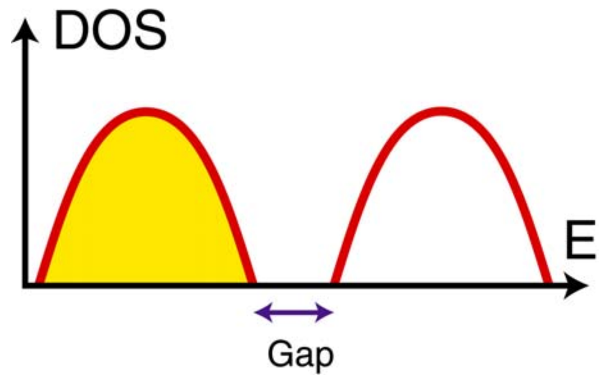
Metal

- Partially filled band
- Finite Density of States (DOS) at Fermi Energy



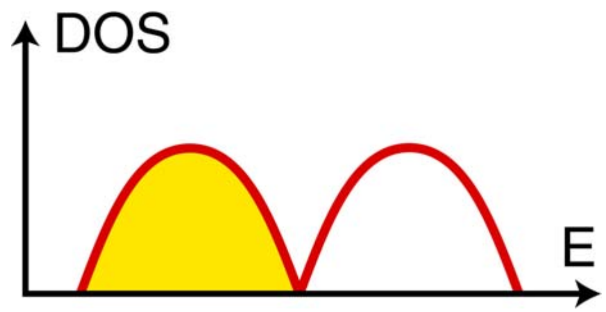
Semiconductor

- Filled Band
- Gap at Fermi Energy

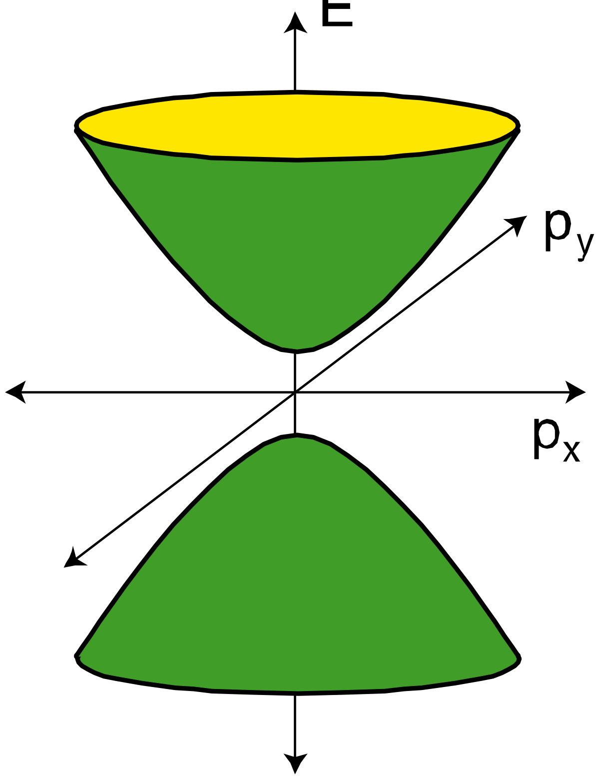


Graphene A critical state

- Zero Gap Semiconductor
- Zero DOS metal



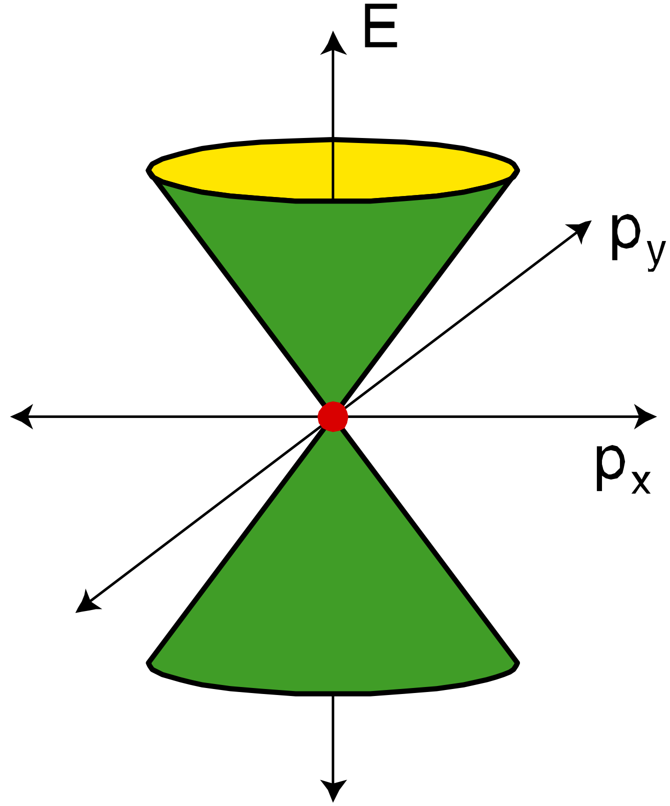
Semiconductor



$$E_c = E_c^0 - \frac{p^2}{2m_c^*}$$

$$E_v = E_v^0 - \frac{p^2}{2m_v^*}$$

Graphene



$$E = \pm v_F \, |\vec{p}\,|$$

"Fermi velocity"

$$v_F = 8\times 10^5 \, m/s$$

Theory of Relativity

A stationary particle (p=0) has rest energy

$$E = mc^2$$

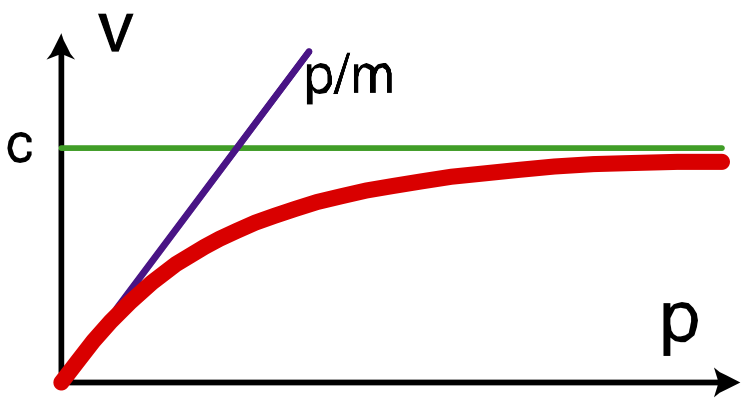
A particle in motion is described by the relativistic dispersion relation:

$$E = \sqrt{(mc^2)^2 + (cp)^2}$$

Albert Einstein 1879-1955

Velocity:

$$\mathrm{v} = \frac{\partial E}{\partial p} = c\frac{cp}{\sqrt{(mc^2)^2 + (cp)^2}}$$

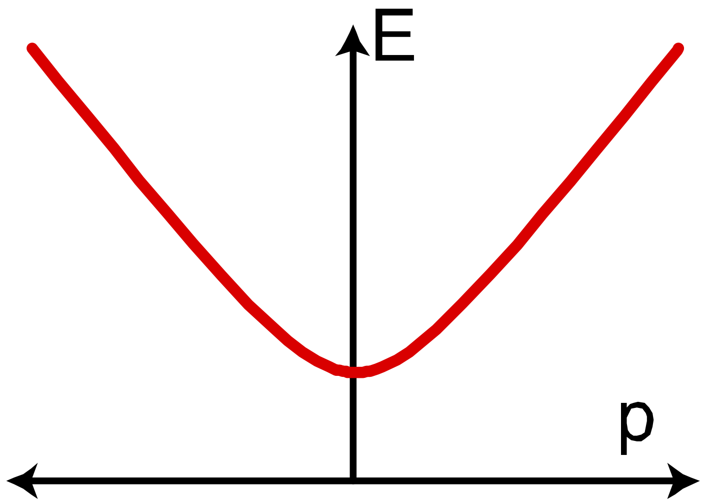


Massive Particle (e.g. electron)

$$E = \sqrt{(mc^2)^2 + (cp)^2}$$

Nonrelativistic limit (v<<c)

$$E \approx mc^2 + \frac{p^2}{2m} + \ldots$$

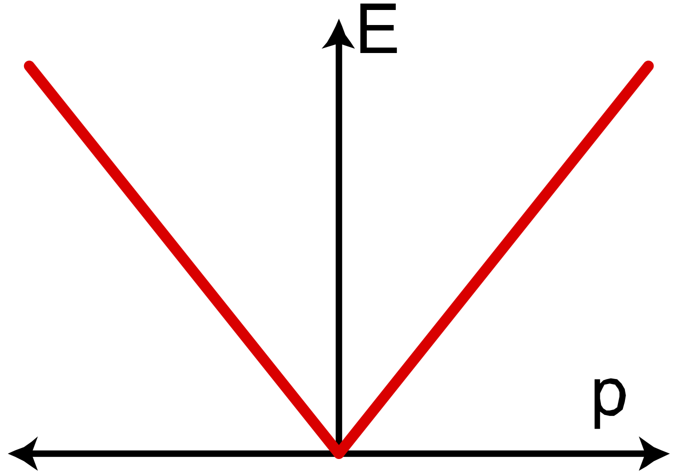


Massless Particle (e.g. photon)

$$m = 0$$

$$E = c\,|\,p\,|$$

$$\mathrm{v} = c$$



Wave Equation

$$E = \hbar\omega \sim i\hbar\frac{\partial}{\partial t} \quad ; \quad \vec{p} = \hbar k \sim -i\hbar\vec{\nabla} \qquad (\text{e.g.} \quad \psi = e^{i(k\bullet r - \omega t)})$$

Non relativistic particles: Schrodinger Equation

$$E = \frac{p^2}{2m} \quad \Rightarrow \quad i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi$$

Relativistic particles: Klein Gordon Equation

$$E^2 = c^2 p^2 + m^2 c^4 \quad \Rightarrow \quad -\hbar^2\frac{\partial^2\psi}{\partial t^2} = (-\hbar^2 c^2 \nabla^2 + m^2 c^4)\psi$$

In order to preserve particle conservation, quantum theory requires a wave equation that is first order in time.

Niels Bohr 1885-1958

Paul Dirac 1902-1984

Niels Bohr : “What are you working on Mr. Dirac?”

Paul Dirac : “I’m trying to take the square root of something”

Dirac's Solution (1928)

How can you take the square root of $p_x^2 + p_y^2 + m^2$ without taking a square root?

$$(p_x^2 + p_y^2 + m^2)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} m & p_x - ip_y \\ p_x + ip_y & -m \end{pmatrix}\begin{pmatrix} m & p_x - ip_y \\ p_x + ip_y & -m \end{pmatrix}$$

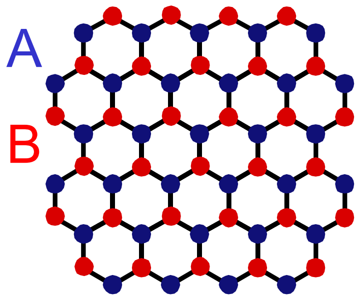
$$\sqrt{(p_x^2 + p_y^2 + m^2)I} = p_x\sigma_x + p_y\sigma_y + m\sigma_z$$

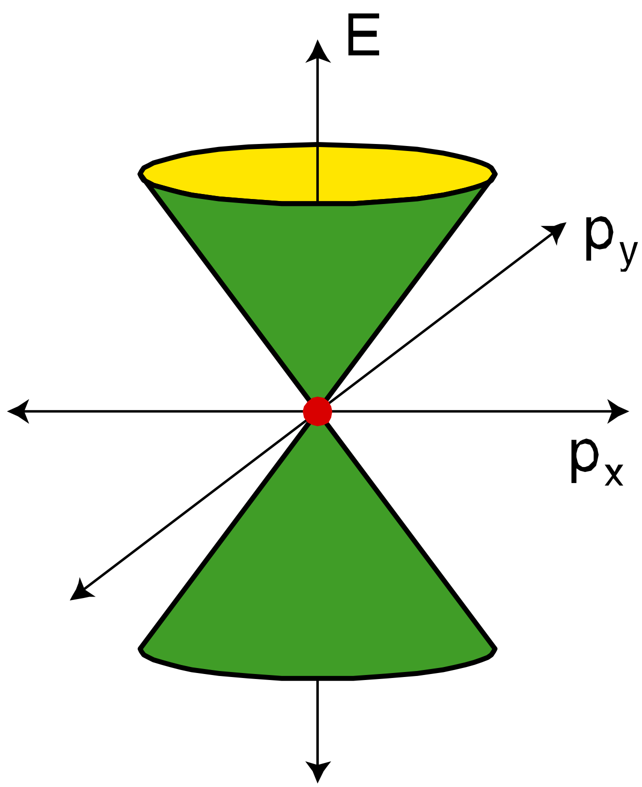
"Dirac Matrices" : $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$; $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$; $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Dirac Equation

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-i\hbar \left(\sigma_x \frac{\partial}{\partial x} + \sigma_y \frac{\partial}{\partial y} \right) + \sigma_z m \right] \psi \qquad \psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Low Energy Electronic Structure of Graphene





The low energy electronic states in graphene are described by the Dirac equation for particles with

Mass : m=0

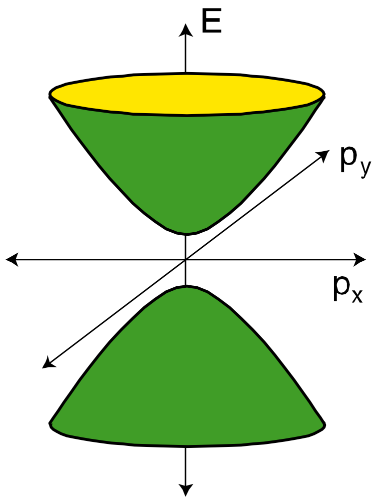
"Speed of light" $c = v_F$

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$ sublattice A / sublattice B

Emergent Dirac Fermions

Consequences of Dirac Equation

1. The existence of Anti Particles



$$E = \pm\sqrt{(mc^2)^2 + (cp)^2}$$

anti electron = positron

Massive Dirac Eq. ~ Semiconductor

Gap 2 $m_e c^2$

Effective Mass $m^* = m_e$

Anti Particles ~ Holes

Consequences of Dirac Equation

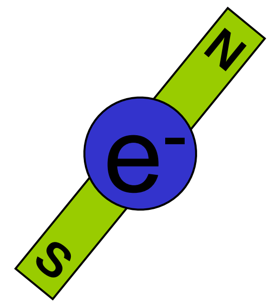
2. The existence of Spin

- Electrons have intrinsic angular momentum

$$J = L + S \qquad S_z = \pm \frac{\hbar}{2}$$

Total a.m. Orbital a.m. Spin a.m.

- Electrons have permanent magnetic moment (responsible for magnetism)

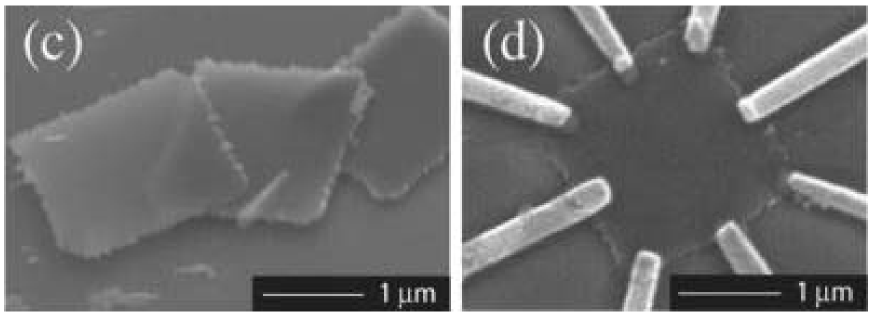


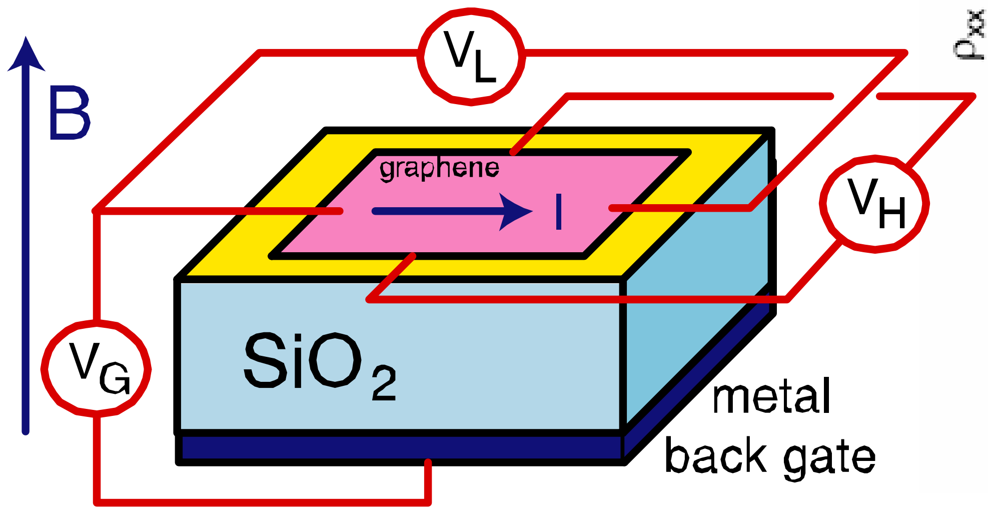
- Interpretation natural for graphene

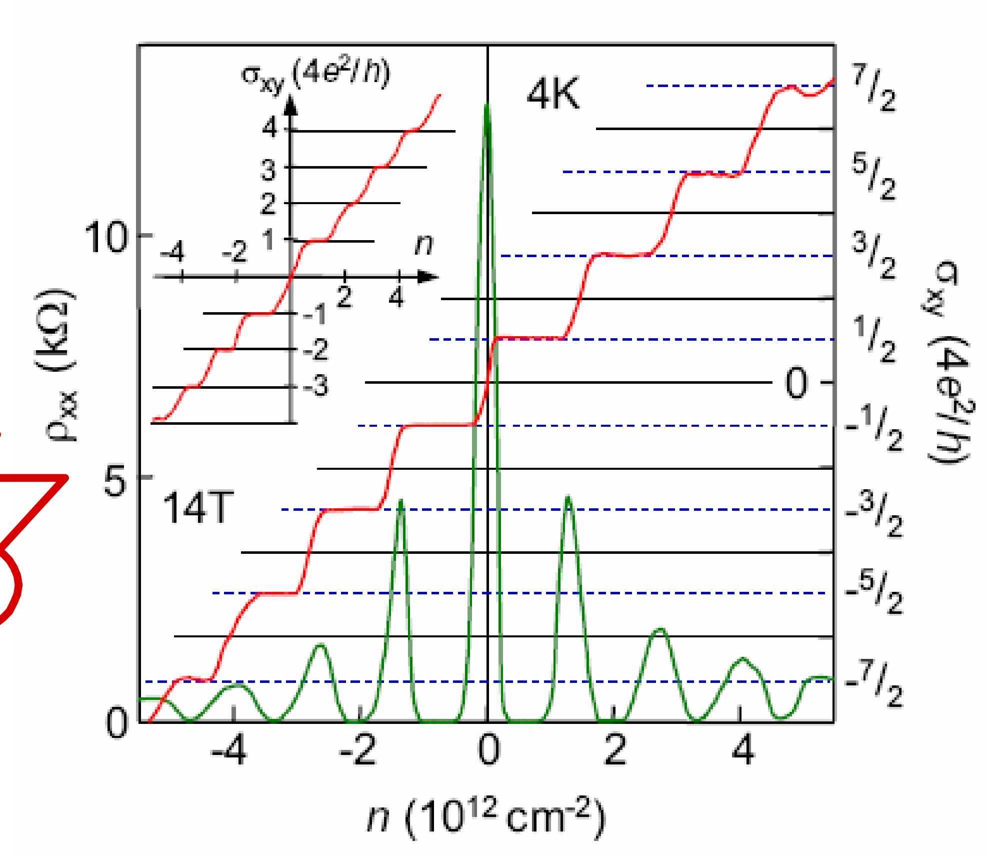
$$\begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \sim \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

"pseudo spin" ~ sublattice index

Experiments on Graphene

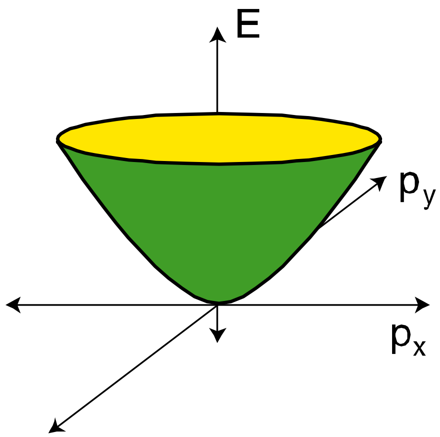


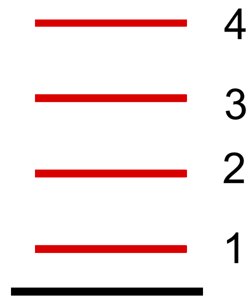




- Gate voltage controls charge n on graphene (parallel plate capacitor)
- Ambipolar conduction: electrons or holes

Landau levels for classical particles

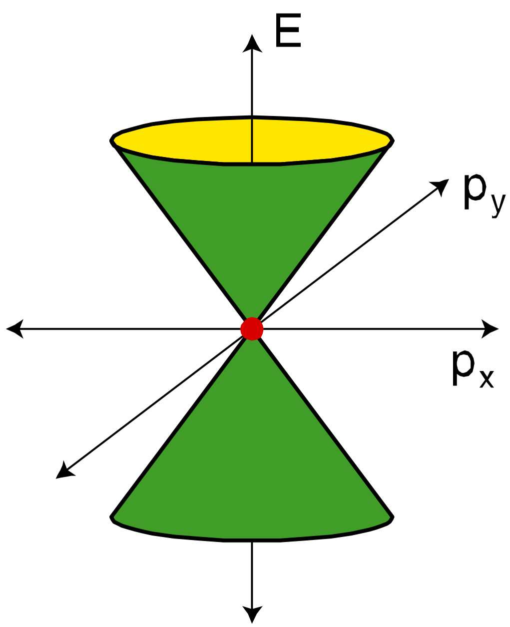


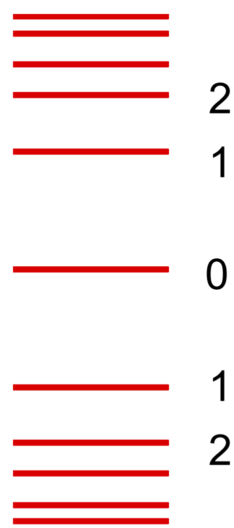


$$E_n = (n + \frac{1}{2}) \frac{\hbar e B}{m}$$

for n=0, 1, 2, ...

Landau levels for relativistic particles





$$E_n = \pm\sqrt{e\hbar v_F^2 B n}$$

for n=0, 1, 2, ...

Existence of landau level at 0 is deeply related to spin in Dirac Eq.