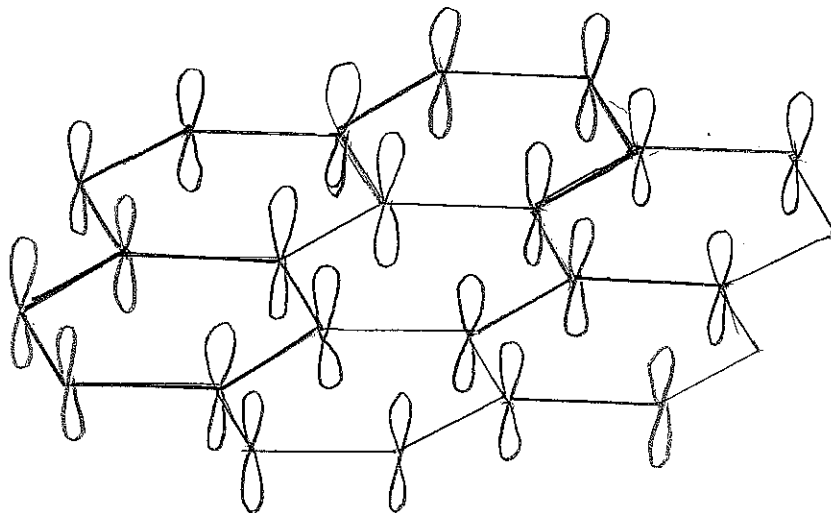


Lecture 11

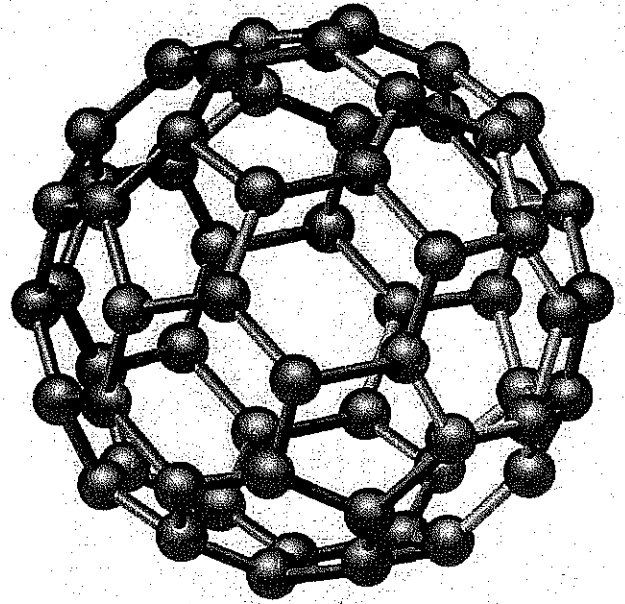
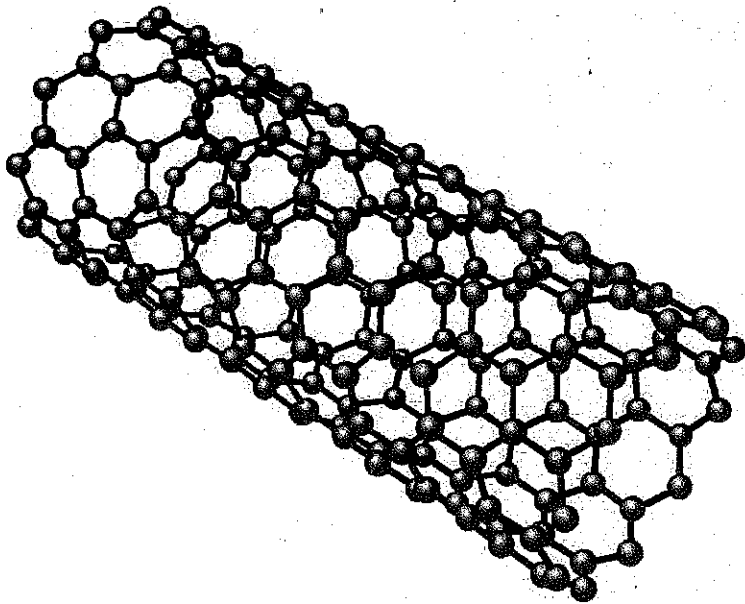
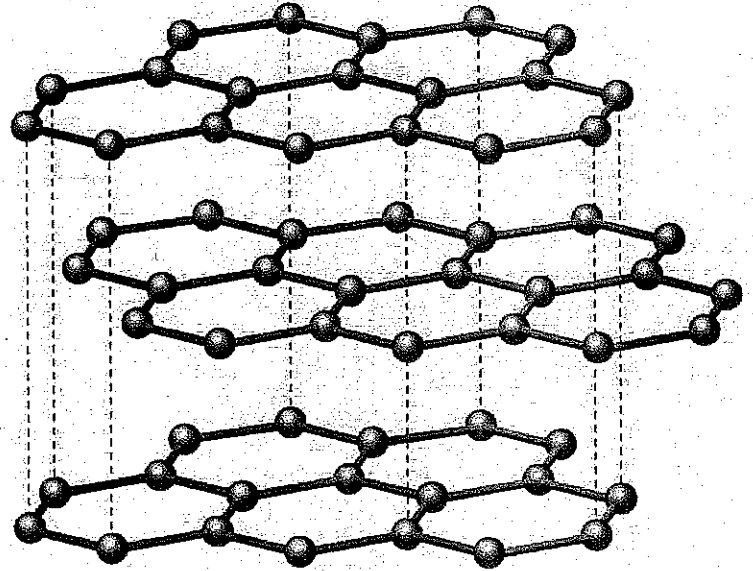
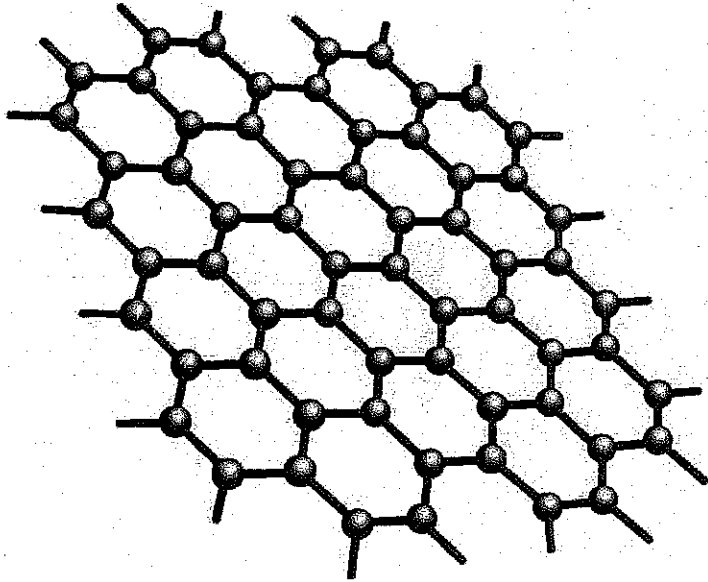
Graphene

Carbon has four valence electrons which occupy $2s^2$ and $2p^2$ orbitals. In diamond there is sp^3 hybridization and four bonds with tetrahedral orientation are formed. In graphene and graphite three valence electrons occupy hybrid sp^2 orbitals to form three very strong covalent σ -bonds that produce hexagonal structure. They are filled electron bands in graphite. The remaining fourth electron for each carbon is in the p_z orbital that is perpendicular to the plane. These orbitals weakly overlap and form narrow band of π -bands.



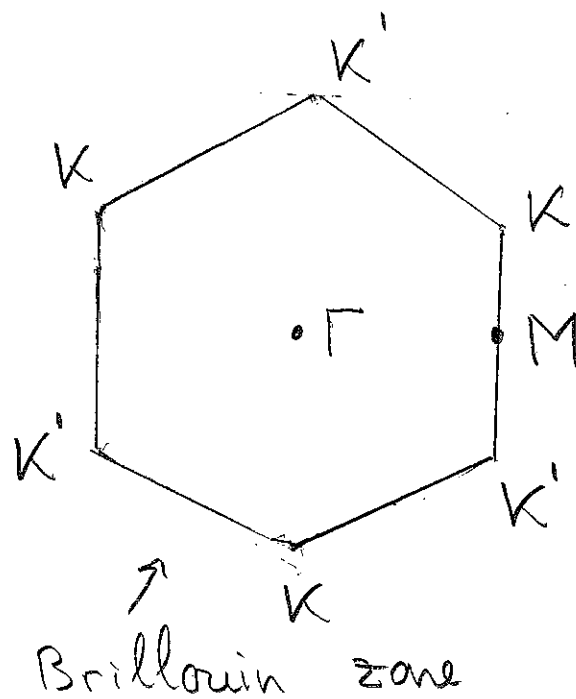
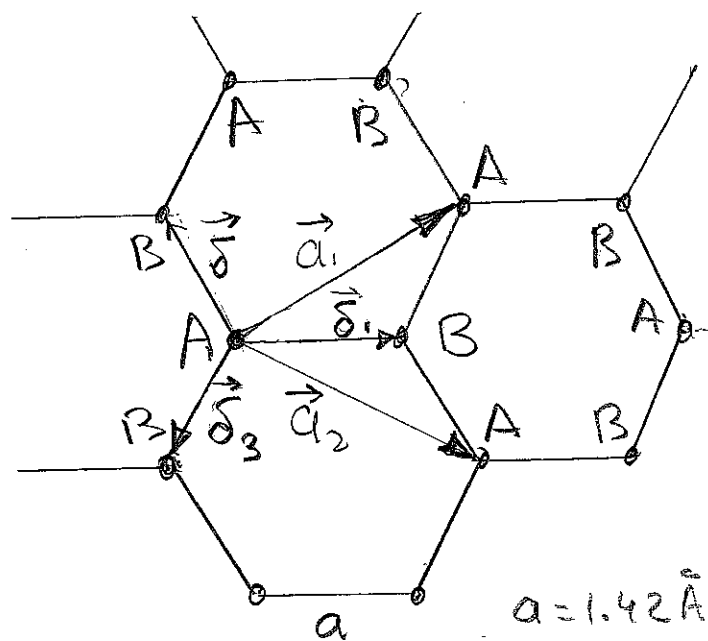
Graphene allotrope

2 Graphene: mother of them all



Graphene (top left) consists of a 2D hexagonal lattice of carbon atoms. Each atom is covalently bonded to three others; but since carbon has four valence electrons, one is left free – allowing graphene to conduct electricity. Other well-known forms of carbon all derive from graphene: graphite is a stack of graphene layers (top right); carbon nanotubes are rolled-up cylinders of graphene (bottom left); and a buckminsterfullerene (C₆₀) molecule consists of graphene balled into a sphere by introducing some pentagons as well as hexagons into the lattice (bottom right).

In graphene the carbon atoms form the honeycomb lattice. The Bravais lattice is hexagonal with two atoms per unit cell: A and B



$$\vec{a}_1 = a \left(\frac{3}{2}, \frac{\sqrt{3}}{2} \right)$$

$$\vec{a}_2 = a \left(\frac{3}{2}, -\frac{\sqrt{3}}{2} \right)$$

reciprocal lattice vectors:

$$\vec{b}_1 = \frac{2\pi}{3a} (1, \sqrt{3})$$

$$\vec{b}_2 = \frac{2\pi}{3a} (1, -\sqrt{3})$$

The honeycomb lattice consists of two shifted hexagonal sublattices made of A and B atoms. In tight binding model with nearest neighbors the hopping is between atoms belonging to the different sublattices $A \leftrightarrow B$

Denoting creation operators of electrons in A and B cells as a_i^+ , b_i^+ we can write the tight binding Hamiltonian

$$H = -t \sum_{i,j=\text{nn}} (a_{i,s}^+ b_{j,s} + b_{j,s}^+ a_{i,s}) \quad t = 2.8 \text{ eV}$$

here sum is over nearest neighbors.

Switching to a Fourier representation we get

$$H = -t \sum_{k,s} \left[\gamma(k) a_{k,s}^+ b_{k,s} + \gamma^*(k) b_{k,s}^+ a_{k,s} \right]$$

$$\text{with } \gamma(k) = \sum_{j=1,2,3} e^{i\vec{k} \cdot \vec{\delta}_j} =$$

$$= e^{i k_x a} + e^{-\frac{i k_x a}{2}} \left(e^{i \frac{\sqrt{3}}{2} k_y a} + e^{-i \frac{\sqrt{3}}{2} k_y a} \right) =$$

$$= e^{i k_x a} \left(1 + 2e^{-\frac{i 3 k_x a}{2}} \cos\left(\frac{\sqrt{3}}{2} k_y a\right) \right)$$

Since each carbon site lacks inversion symmetry $\gamma(k)$ is complex.

One can rewrite it in the matrix form

(5)

$$M = \sum_{\mathbf{k}, S} \begin{pmatrix} a_{\mathbf{k}, S}^+ & b_{\mathbf{k}, S}^+ \\ a_{\mathbf{k}, S} & b_{\mathbf{k}, S} \end{pmatrix} \begin{pmatrix} 0 & \pm \gamma(\mathbf{k}) \\ \pm \gamma^*(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}, S} \\ b_{\mathbf{k}, S} \end{pmatrix}$$

Diagonalizing $M \hat{\Psi} = \epsilon \hat{\Psi}$ we obtain the eigenvalues

$$\epsilon(\mathbf{k}) = \pm t |\gamma(\mathbf{k})| =$$

$$= \pm t \sqrt{1 + 4 \cos\left(\frac{3}{2} k_x a\right) \cos\left(\frac{\sqrt{3}}{2} k_y a\right) + 4 \cos^2\left(\frac{\sqrt{3}}{2} k_y a\right)}$$

Let's analyze this spectrum

At the Γ point ($\mathbf{k}=0$) and $\epsilon(\mathbf{k}=0) = \pm 3t$

For six M points $\mathbf{K}_M = \pm \frac{2\pi}{3a} (1, 0)$ $\epsilon(\mathbf{K}_M) = \pm t$

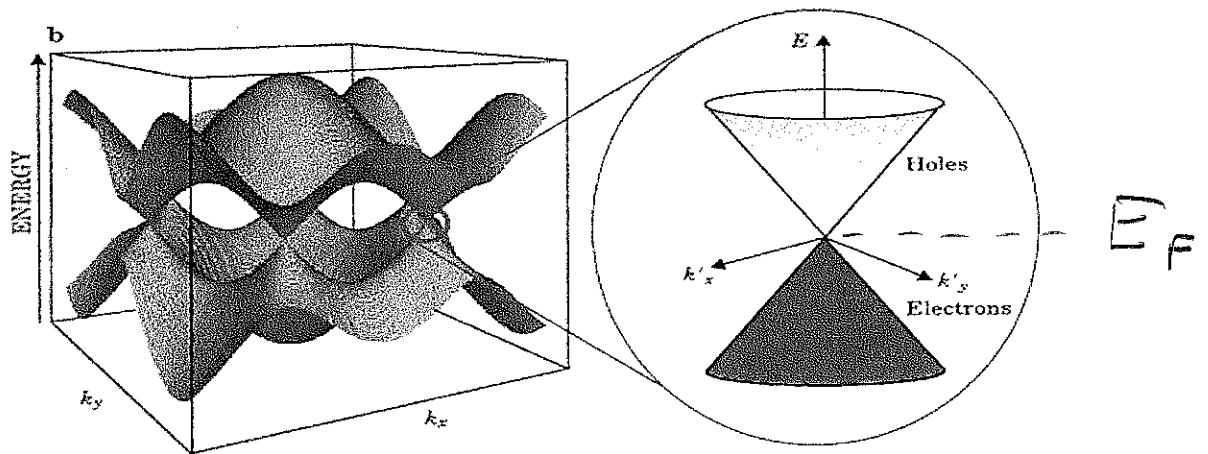
For three K points $\mathbf{K}_K = \frac{4\pi}{3\sqrt{3}a} (0, -1), \frac{4\pi}{3\sqrt{3}a} \left(\pm \frac{\sqrt{3}}{2}, \frac{1}{2}\right)$

$$\gamma_{\mathbf{K}} = 0. \quad \epsilon(\mathbf{K}_K) = 0.$$

The same happens at three \mathbf{K}' points

At these points two branches with \pm signs have the same energy. $\epsilon(\mathbf{k}) = 0$

Band structure:



These K and K' points are called Dirac points. It is important that K and K' are not connected by a reciprocal lattice vector, they are independent values of \vec{k} . In the absence of doping graphene has exactly one electron per atom \equiv 2 per unit cell, half filling. Then the Fermi energy $E_F = 0$ and the Fermi surface shrinks to the point. Undoped graphene is a perfect semimetal.

Let us calculate the energy spectrum near a Dirac point $\vec{k} = \vec{K}_K + \vec{p}$

$$\begin{aligned} \gamma &= e^{-i\vec{p} \cdot \vec{a}} \left(1 + 2e^{-i\frac{3}{2}\vec{p}_x a} \cos\left(-\frac{2\pi}{3} + \frac{\sqrt{3}}{2}\vec{p}_y a\right) \right) = \\ &= 1 + 2\left(1 - i\frac{3}{2}\vec{p}_x a\right) \left(-\frac{1}{2} + \frac{\sqrt{3}}{2} \frac{\sqrt{3}}{2}\vec{p}_y a\right) = \frac{3}{2}a(i\vec{p}_x + \vec{p}_y) \end{aligned}$$

Taking phase factor i out we arrive at the Dirac Hamiltonian

$$H = \hbar v_F \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} = \hbar v_F \vec{\sigma} \cdot \vec{p}, \quad \epsilon(p) = \pm v_F |p|$$

where $\vec{\sigma}$ are Pauli matrices and

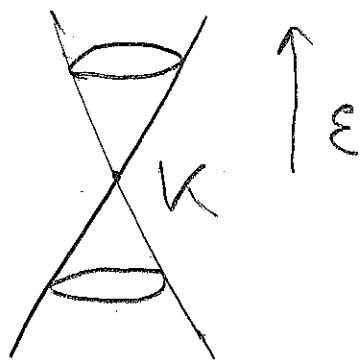
$v_F = \frac{3ta}{2\hbar} \cong 10^6 \text{ m/sec}$ replaces the light velocity.

Density of states

$$N(E) = \frac{2}{(2\pi\hbar)^2} \int_{\epsilon=E} \frac{dS}{|\partial\epsilon/\partial p|}$$

For small energies we have $\epsilon = v_F |p|$

$$\text{and } N(E) = \frac{2}{(2\pi\hbar)^2} \frac{2\pi E}{v_F^2} = \frac{E}{\pi(\hbar v_F)^2}$$



Cyclotron mass

One can "dope" graphene by applying a gate voltage. Then we will get a Fermi surface and the carrier density

$$n_s = \frac{P_F^2}{\pi \hbar^2}$$

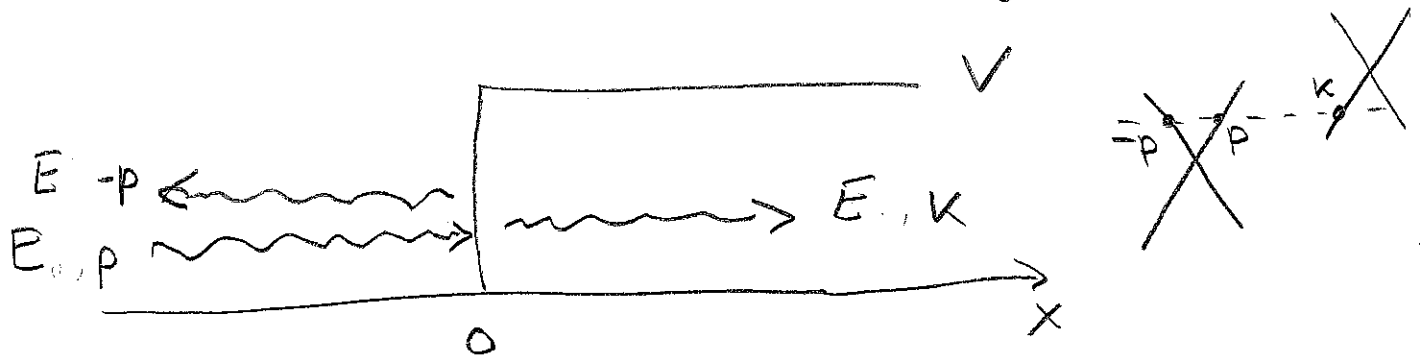
Effective mass is given by

$$m^* = \frac{P_F}{|\partial E / \partial p|_{P_F}} = \frac{P_F}{v_F} = \frac{\sqrt{\pi} \hbar \sqrt{n_s}}{v_F}$$

This mass can be measured in the cyclotron resonance experiments.

Klein tunneling

Massive particle cannot live under the barrier. This is not the case for Dirac electron. Consider the following geometry



We should solve equation

$$(\partial_x p + V(x)) \psi = E \psi \quad V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x > 0 \end{cases}$$

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

$$-i \frac{\partial \psi_1}{\partial x} = (E - V(x)) \psi_2$$

$$\text{Solution: } \psi_r = A e^{ipx} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + A' e^{-ipx} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$p = E, \quad x < 0.$$

$$\text{and } \psi_t = B e^{ikx} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad k = E - V_0$$

matching these wave functions at $x=0$

$$\psi_r(0) = \psi_t(0) \text{ gives } A' = 0, \quad A = B \text{ and}$$

transmission coefficient $t = 1$.

Landau levels

In a magnetic field we replace p by $p - \frac{e\hbar}{c}$

Then our Dirac Eq. is

$$U_F \gamma \cdot (-i\vec{\nabla} - \frac{e\vec{A}}{c}) \psi(r) = E \psi(r)$$

we choose gauge $A(r) = B(y, 0, 0)$

We are looking for the wave function

$$\psi(x, y) = e^{ik_x x} f(y)$$

$$U_F \begin{pmatrix} 0 & k_x - \frac{Be y}{c} + \frac{\partial}{\partial y} \\ k_x - \frac{Be y}{c} - \frac{\partial}{\partial y} & 0 \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = E \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$

Introducing $y_0 = \frac{k_x}{eB}$ we obtain

$$U_F \frac{eB}{c} \begin{pmatrix} 0 & y - y_0 + \frac{c}{eB} \frac{\partial}{\partial y} \\ y - y_0 - \frac{c}{eB} \frac{\partial}{\partial y} & 0 \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = E \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$

$$H = \frac{U_F}{l^2} \begin{pmatrix} 0 & y - y_0 + l^2 \frac{\partial}{\partial y} \\ y - y_0 - l^2 \frac{\partial}{\partial y} & 0 \end{pmatrix}$$

where $l = \left(\frac{c}{eB}\right)^{1/2}$ is magnetic length

The off diagonal terms are harmonic oscillator operators

$$a = \frac{1}{\sqrt{2}} \left(\frac{z}{z_0} + \frac{\partial}{\partial \frac{z}{z_0}} \right), \quad a^\dagger = \frac{1}{\sqrt{2}} \left(\frac{z}{z_0} - \frac{\partial}{\partial \frac{z}{z_0}} \right)$$

$$\frac{z}{z_0} = \frac{y - y_0}{e}$$

$$H\psi = \frac{\sqrt{2} U_F \hbar}{e} \begin{pmatrix} 0 & a \\ a^\dagger & 0 \end{pmatrix} \begin{pmatrix} |n-1\rangle \\ |n\rangle \end{pmatrix}$$

here $|n\rangle$ are harmonic oscillator states

Equating $H\psi = E\psi$ and using

$a^\dagger |n-1\rangle = \sqrt{n}$ we obtain

$$E = \pm \sqrt{2} \hbar \frac{U_F}{e} \sqrt{n} = \pm \sqrt{2} \hbar U_F \left(\frac{eB}{c} \right)^{1/2} n^{1/2}$$

quite different from the usual Landau level quantization

$$E = \omega_c \left(n + \frac{1}{2} \right) = \frac{eB}{mc} \left(n + \frac{1}{2} \right)$$