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

- Diamond
- Graphene = A single layer of graphite
- C_{60} "buckminsterfullerene"
- Graphite
- (10,10) tube

1.4 Å ↔ graphite
3.4 Å
Graphene Electronic Structure

Carbon: $Z=6$ ; 4 valence electrons

- $1s$ (2 states)
- $2s, 2p$ (8 states)
- $3s, 3p, 3d$ (18 states)

**$sp^2$ bonding**

- $\sigma$ bonds: exceptional structural rigidity
- $\pi$ electrons: allow conduction

$\pi$ orbital ($\perp$ to plane) derived from $p_z$

$\sigma$ orbital (in plane) derived from $s$, $p_x$, $p_y$
Hopping on the Honeycomb

π

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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Hopping on the Honeycomb

π

Textbook QM problem: Tight binding model on the Honeycomb lattice

sublattice A
sublattice B
unit cell

Just like CJ’s homework!

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

Graphene

\[ E_c = E^0_c - \frac{p^2}{2m^*_c} \]

\[ E_v = E^0_v - \frac{p^2}{2m^*_v} \]

\[ E = \pm v_F | \vec{P} | \]

“Fermi velocity”

\[ v_F = 8 \times 10^5 \text{ m/s} \]
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:

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

Velocity:

\[ v = \frac{\partial E}{\partial p} = c \frac{cp}{\sqrt{(mc^2)^2 + (cp)^2}} \]
Massive Particle (e.g. electron)

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

Nonrelativistic limit (\( v \ll c \))

\[ E \approx mc^2 + \frac{p^2}{2m} + ... \]

Massless Particle (e.g. photon)

\[ m = 0 \]

\[ E = c |p| \]

\[ v = c \]
Wave Equation

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

Non relativistic particles: Schrödinger 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: “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

$$\frac{i\hbar}{\partial t} = \begin{Bmatrix} -i\hbar \left( \sigma_x \frac{\partial}{\partial x} + \sigma_y \frac{\partial}{\partial y} \right) + \sigma_z m \end{Bmatrix} \psi$$

$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$
The low energy electronic states in graphene are described by the Dirac equation for particles with

\[ \psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \]

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
  \[ J = L + S \]
  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” \sim 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

\[ E_n = \left(n + \frac{1}{2}\right) \frac{\hbar e B}{m} \]

for \( n = 0, 1, 2, \ldots \)

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

Landau levels for relativistic particles

\[ E_n = \pm \sqrt{\hbar v_F^2 B n} \]

for \( n = 0, 1, 2, \ldots \)