Aspects of Dirac Physics in Graphene

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Overview

1. Origin of Dirac physics in graphene
2. Superconducting junctions
3. Physics of graphene junctions
4. Kondo physics and STM spectroscopy in graphene
5. Conclusion
Origin of Dirac physics in graphene
Relevant Basics about graphene

Honeycomb lattice

Tight binding model for graphene with nearest neighbor hopping.

Can in principle include next-nearest neighbor hopping: same low energy physics. Ref: arXiv:0709.1163

Each unit cell has two electrons from $2p_z$ orbital leading to delocalized $\pi$ bond.

$$H = \int d^2x \psi^\dagger \begin{pmatrix} 0 & \hat{t} \\ \hat{t} & 0 \end{pmatrix} \psi$$

$$\psi = (\psi_A, \psi_B)$$
Diagonalize in momentum space to get the energy dispersion.

\[
H = \int d^2k \psi^\dagger(k) \begin{pmatrix} 0 & h(k) \\ h^*(k) & 0 \end{pmatrix} \psi(k)
\]

\[
h(k) = -t \sum_{j=1}^{3} e^{-i k \cdot \tau_j}
\]

Energy dispersion: \( E_{\pm}(k) = \pm E(k) = \pm |h(k)| \)
There are two energy bands (valence and conduction) corresponding to energies $\pm E(k)$. These two bands touch each other at six points at the edges of the Brillouin zone. Two of these points K and K' are inequivalent; rest are related by translation of a lattice vector. Two inequivalent Fermi points rather than a Fermi-line. Dirac cone about the K and K' points. $E(k) \sim \pm v_F |k|$. 

\[ E(k) \sim \pm v_F |k| \]
Thus at low energies one can think of a four component wave function for the low-energy quasiparticles (sans spin).

\[ \psi = (\psi_A^K, \psi_B^K, \psi_A^{K'}, \psi_B^{K'}) \]

<table>
<thead>
<tr>
<th>Terminology</th>
<th>Pauli matrix</th>
<th>Relevant space</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pseudospin</td>
<td>( \sigma )</td>
<td>2 by 2 matrix associated with two sublattice structure</td>
</tr>
<tr>
<td>Valley</td>
<td>( \tau )</td>
<td>2 by 2 matrix associated with two BZ points K and K'</td>
</tr>
<tr>
<td>Spin</td>
<td>( S )</td>
<td>2 by 2 matrix associated with the physical spin.</td>
</tr>
</tbody>
</table>

At each valley, we have a massless Dirac eqn. with Dirac matrices replaced by Pauli matrices and \( c \) replaced by \( v_F \).

No large \( k \) scattering leads to two species of massless Dirac Fermions.
Helicity associated with Dirac electrons at $K$ and $K'$ points.

Solution of $H_a$ about $K$ point:

$$\psi_K \simeq (1, \pm e^{i\gamma})$$
$$\gamma = \tan^{-1}(k_y/k_x)$$

Electrons with $E>0$ around $K$ point have their pseudospin along $k$ where pseudospin refers to A-B space. For $K'$, pseudospin points opposite to $k$.

$E_F$ can be tuned by an external gate voltage.

DOS varies linearly with $E$ for undoped graphene but is almost a constant at large doping. $\rho(E) \sim |E - E_F|$
Simple Problem: What is the probability of the incident electron to penetrate the barrier?

**Solve the Schrödinger equation and match the boundary conditions**

**Answer:**

\[ T = |t|^2 = \frac{4\chi^2 k^2}{4\chi^2 k^2 + (k^2 + \chi^2)^2 \sinh^2(\chi)} \]

where

\[ \chi = \frac{2(V_0 - E)d}{\hbar v_d}, \quad v_d = \frac{\hbar}{md}, \quad k^2 = \frac{2md^2 E}{\hbar^2} \]

**Basic point:** For \( V_0 \gg E \), \( T \) a monotonically decreasing function of the dimensionless barrier strength.
Simple QM 102: A 2D massless Dirac electron in a potential barrier


For any angle of incidence $T=1$ if $\tan(\gamma) = k_y/k_x$.

Basic point: $T$ is an oscillatory function of the dimensionless barrier strength. Qualitatively different physics from that of the Schrödinger electrons.

$T_D = |t|^2 = \frac{\cos^2(\gamma)}{1 - \cos^2(\chi) \sin^2(\gamma)}$

$\chi = \frac{V_0 d}{\hbar v_F}$

Conventional Superconducting junctions
Superconductivity and tunnel junctions

Measurement of tunneling conductance

N-I-N interface

N-I-S interface

Insulator (I)

Normal metal (N)

Superconductor (S)

$E_{FN}^L$

$E_{FN}^R$

$E_{FS}$

$\Delta_0$

$eV$
Basic mechanism of current flow in a N-I-S junction

Andreev reflection is strongly suppressed in conventional junctions if the insulating layer provides a large potential barrier: so called tunneling limit.

In conventional junctions, subgap tunneling conductance is a monotonically decreasing function of the effective barrier strength $Z$.

Zero bias tunneling conductance decays as $1/(1+2z^2)^2$ with increasing barrier strength.

BTK, PRB, 25 4515 (1982)
Josephson Effect

The ground state wavefunctions have different phases for $S_1$ and $S_2$:

$\psi_1 \sim e^{i\phi_1}$

$\psi_2 \sim e^{i\phi_2}$

Thus one might expect a current between them: DC Josephson Effect

$j \sim \text{Im}[\psi_1^* \psi_2] \sim \sin(\phi_2 - \phi_1)$

Experiments: Josephson junctions [Likharev, RMP 1979]

S-N-S junctions or weak links

S-B-S or tunnel junctions
Josephson effect in conventional tunnel junctions

Formulation of localized subgap Andreev bound states at the barrier with energy dispersion which depends on the phase difference of the superconductors.

The primary contribution to Josephson current comes from these bound states.

Kulik-Omelyanchuk limit:

\[ T \to 1 \quad I(T_0 = 0) \sim |\sin(\phi/2)| \]
\[ I_c R_N = \pi \Delta_0 / e \]

Ambegaokar-Baratoff limit:

\[ T \to 0 \quad I(T_0 = 0) \sim T \sin(\phi) \]
\[ I_c R_N = \pi \Delta_0 / 2e \]

Both \( I_c \) and \( I_c R_N \) monotonically decrease as we go from KO to AB limit.
Graphene Junctions
Graphene N-B-S junctions

Superconductivity is induced via proximity effect by the electrode.

Effective potential barrier created by a gate voltage $V_g$ over a length $d$. Dimensionless barrier strength: $\chi = V_g d / (\hbar v_F)$

Applied bias voltage $V$.

Dirac-Bogoliubov-de Gennes (DBdG) Equation

$$
\begin{pmatrix}
\mathcal{H}_a - E_F + U(r) & \Delta(r) \\
\Delta^*(r) & E_F - U(r) - \mathcal{H}_a
\end{pmatrix}
\begin{pmatrix}
\psi_a \\
\psi_a
\end{pmatrix} = E
\begin{pmatrix}
\psi_a \\
\psi_a
\end{pmatrix}
$$

$E_F$ → Fermi energy
$U(r)$ → Applied Potential = $V_g$ for $0 > x > -d$
$\nabla r$ → Superconducting pair-potential between electrons and holes at K and K' points

Question: How would the tunneling conductance of such a junction behave as a function of the gate voltage?
Central Result: In complete contrast to conventional NBS junction, Graphene NBS junctions, due to the presence of Dirac-like dispersion of its electrons, exhibit novel periodic oscillatory behavior of subgap tunneling conductance as the barrier strength is varied.

- Periodic oscillations of subgap tunneling conductance as a function of barrier strength

\[ \chi = \frac{n+1}{2} \]

Tunneling conductance maxima occur at \[ \chi = \frac{n+1}{2} \]
Transmission resonance condition

Maxima of conductance occur when \( r=0 \).

For subgap voltages, in the thin barrier limit, and for \( eV \ll E_F \), it turns out that

\[
G = G_0 \int_0^{k_F} \frac{dk_{||}}{2\pi} \left( 1 - |r|^2 + |r_A|^2 \right)
\]

where \( r = \sin(\gamma) \cos(\chi) \sin(\beta) \),

1. \( \beta = 0 \): Manifestation of Klein Paradox. Not seen in tunneling conductance due to averaging over transverse momenta.

2. \( \beta = 0 \): Maxima of tunneling conductance at the gap edge: also seen in conventional NBS junctions.

3. \( \beta = (n+1/2) \beta \): Novel transmission resonance condition for graphene NBS junction.
Oscillations persists: so one expects the oscillatory behavior both as functions of $V_G$ and $d$ to be robust.

However, the maximum value of $G$ may be lesser than the Andreev limit value of $2G_0$.

The periodicity of the oscillations shall vary with $V_G$ and will deviate from $\tau_0$. 

Not so thin barrier
Graphene S-B-S junctions

Schematic Setup

Question: How would the Josephson current behave as a function of the gate voltage $V_0$?

Procedure:
1. Solve the DBdG equation in regions I, II and B.
2. Match the boundary conditions at the boundaries between regions I and B and B and II.
3. Obtain dispersion for bound Andreev subgap states and hence find the Josephson current.

$$
\begin{pmatrix}
\mathcal{H}_a - E_F + U(r) & \Delta(r) \\
\Delta^*(r) & E_F - U(r) - \mathcal{H}_a
\end{pmatrix}
\begin{pmatrix}
\psi_a \\
\psi_a
\end{pmatrix}
= E
\begin{pmatrix}
\psi_a \\
\psi_a
\end{pmatrix}
$$

- $E_F$ : Fermi energy
- $U(r)$ : Applied Potential $= V_0$ for $0>x>-d$
- $\Delta(r)$ : Superconducting pair-potential in regions I and II as shown
DBdG quasiparticles has a transmission probability $T$ which is an oscillatory function of the barrier strength. 

The Josephson current is an oscillatory function of the barrier strength $\phi$.

$$
\epsilon_{\pm}(q, \phi; \chi) = \pm \Delta_0 \sqrt{1 - T(\gamma, \chi) \sin^2(\phi/2)},
$$

$$
T(\gamma, \chi) = \frac{\cos^2(\gamma)}{1 - \cos^2(\chi) \sin^2(\gamma)}.
$$

$$
\sin(\gamma) = \hbar \nu F q / E_F.
$$

$$
I(\phi, \chi, T_0) = I_0 g(\phi, \chi, T_0)
$$

$$
g(\phi, \chi, T_0) = \int_{-\pi/2}^{\pi/2} d\gamma \left[ \frac{T(\gamma, \chi) \cos(\gamma) \sin(\phi)}{\sqrt{1 - T(\gamma, \chi) \sin^2(\phi/2)}} \right] \times \tanh(\epsilon_+/2k_B T_0).
$$
$I_c$ and $I_cR_N$ are periodic bounded oscillatory functions of the effective barrier strength $\tau$.

$I_cR_N$ is bounded with values between $\frac{\tau_0}{e}$ for $\tau=n\tau_0$ and $2.27\frac{\tau_0}{e}$ for $\tau=(n+1/2)\tau_0$.

For $\tau=n\tau_0$, $I_cR_N$ reaches $\frac{\tau_0}{e}$: Kulik-Omelyanchuk limit.

Due to transmission resonance of DBdG quasiparticles, it is not possible to make $T$ arbitrarily small by increasing gate voltage $V_0$. Thus, these junctions never reach Ambegaokar-Baratoff limit.
Kondo Physics and STM spectroscopy
Kondo effect in conventional systems

Formation of a many-body correlated state below a crossover temperature $T_K$, where the impurity spin is screened by the conduction electrons.

**Metal + Magnetic Impurity**

**Features of Kondo effect:**

1. Appropriately described by the Kondo model:

   $$ H = H_0 + JS \cdot \mathbf{s}(0) $$


3. For two or more channels of conduction electrons (multichannel) the resultatnt ground state is a non-Fermi liquid. For a single channel, the ground state is still a Fermi liquid.

4. All the results depend crucially on the existence of constant DOS at $E_F$.

5. Kondo state leads to a peak in the conductance at zero bias, as measured by STM.
What’s different for possible Kondo effect in graphene

For undoped graphene, linearly varying DOS makes a Kondo screened phase impossible [Casselano and Fradkin, Ingersent, Polkovnikov, Sachdev and Vojta]. At finite and large doping, an effectively constant DOS occurs and hence one should see a Kondo screened phase.

One can tune into a Kondo screened phase by applying a gate voltage

\[ k_B T^* = \Lambda \exp\left[\frac{(1 - J_c(0)/J)}{(2q \ln[1/q^2])}\right]. \]

\[ q = \frac{eV}{\Lambda}. \]

\( J \approx 2 \text{ eV} \) and voltage \( eV \approx 0.5 \text{ eV} \), \( T^* \approx 35 \text{ K} \).

Also, two species of electrons from \( K \) and \( K' \) points may act as two channels if the impurity radius is large enough so that large-momenta scatterings are suppressed.

Possibility of two-channel Kondo effect in graphene.

Theoretical prediction: Sengupta and Baskaran PRB (2007)
Recent STM experiments on doped graphene

Constant current STM topography of pure graphene (100 nm$^2$ I=40pA)

Adding Cobalt impurity in graphene

There is no experimental control over the position of these cobalt atoms.

The position of these atoms can be accurately determined by STM topography

Typical parameters: $E_F=250$ meV and $T=4$ K.

Observation of Kondo peak in doped graphene sample with \( T_K = 16 \text{K} \)

Proof of two-channel character of the Kondo state: non-Fermi liquid ground state in graphene.
Bimodal Spectra for the Conductance $G$

Impurity at the center: peaked structure of $G$ and 2CK effect

Impurity on site: dip structure of $G$ and 1CK effect

No analog in conventional Kondo systems: property of Dirac electrons
Theory of STM spectra in graphene

Model Hamiltonians for Graphene, Impurity and STM tip

\[
H_G = \int_k \psi^\beta_\gamma^\dagger(\vec{k}) [\hbar v_F (\tau_z \sigma_x k_x + \sigma_y k_y) - E_F I] \psi^\beta_\gamma(\vec{k})
\]

\[
H_d = \sum_{s=\uparrow,\downarrow} \epsilon_d d^\dagger_s d_s + U n_\uparrow n_\downarrow
\]

\[
H_t = \sum_\nu \left[ \sum_{\sigma=\uparrow,\downarrow} \epsilon_{\nu\sigma} t^\dagger_{\nu\sigma} t_{\nu\sigma} + (\Delta_0 t^\dagger_{\nu\uparrow} t^\dagger_{-\nu\downarrow} + h.c) \right] \tag{2}
\]
Tunneling current

Interaction between the tip, impurity and graphene: Anderson model

Tunneling current is derived from the rate of change of number of tip electrons

Obtain an expression for the current using Keldysh perturbation theory
Turn the crank and obtain a formula for the current

Wingreen and Meir (1994)

Contribution from undoped graphene

Impurity contribution

Shape of the spectra depends crucially on the Fano factor $q$ and hence on $W^0/U^0$

What determines the coupling of Dirac electrons to the STM tip?

\[
I = I_0 \int_{-\infty}^{\infty} d\omega \left[ f(\omega - eV) - f(\omega) \right] \rho_t(\omega - eV) \left[ \rho_G(\omega) \times |U^0|^2 + \frac{|B(\omega)|^2 |q(\omega)|^2 - 1 + 2\text{Re}[q(\omega)]\chi(\omega)}{\text{Im}\Sigma_d(\omega)} \right] \]

\[
q(\epsilon) = \frac{[W^0/U^0 + V^0I_1(\epsilon)]/[V^0I_2(\epsilon)]}{[V^0I_2(\epsilon)]},
\]

\[
I_1(\epsilon) = -4(1 + \xi^2)(\epsilon + E_F) \ln \left| 1 - \Lambda^2/(\epsilon + E_F)^2 \right| / \Lambda^2
\]

\[
I_2(\epsilon) = 4(1 + \xi^2)\pi |\epsilon + E_F| \theta(\Lambda - \epsilon - E_F)/\Lambda^2.
\]

\[
B(\epsilon) = V^0U^0I_2(\epsilon)
\]

$U^0$ coupling of graphene to tip

$W^0$ coupling of impurity to tip

$V^0$ coupling of graphene to impurity
What determines $U^0$

Bardeen Tunneling formula

\[ U^0 \sim \int d^2r \left( \phi^\dagger(z) \partial_z \Psi_G(\vec{r}, z) - \Psi_G^\dagger(\vec{r}, z) \partial_z \phi(z) \right) \sim \Psi_G(\vec{r}_0, z_0) \]

Tight-binding wave-function for graphene electrons

\[ \Psi_G(\vec{r}, z) = \frac{1}{\sqrt{N}} \sum_{\vec{R}^A_i} e^{i[\vec{K} + \vec{\delta k} \cdot \vec{R}^A_i]} \left[ \varphi(\vec{r} - \vec{R}^A_i) + e^{+(-i\delta k)} \varphi(\vec{r} - \vec{R}^B_i) \right] f(z). \quad (1) \]

Plane-wave part  
Localized $p_z$ orbital part

Impurity on hexagon center

$U^0$ becomes small leading to large $q$.

\[ q(\epsilon) = \frac{[W^0/U^0 + V^0 I_1(\epsilon)]/[V^0 I_2(\epsilon)]}{\text{Peaked spectra for all values of } E_F \text{ independent of the applied voltage}} \]

Conductance spectra shows a peak for center impurities
**Impurity on Graphene site**

Asymmetric position: No cancelation and $U^0$ remains large

\[
q(\epsilon) = \frac{[W^0/U^0 + V^0 I_1(\epsilon)]/[V^0 I_2(\epsilon)]}{\sim I_1/I_2 \sim -\ln|1 - \Lambda^2/(eV + E_F)^2|/\pi}.
\]

$G$ should exhibit a change from peak to a dip through an anti-resonance with change of $E_F$

Refs: 
- Saha et al (2009)
- Wehling et al (2009)
- Uchoa et al (2009)

**Impurity on hexagon center**

Should be observed on surfaces of topological insulators
Conclusion

1. The field of graphene has shown unprecedented progress over the last few years. First example of so called “Dirac materials”.

2. Several interesting physics phenomenon:
   a) Dirac physics on a tabletop.
   b) Unconventional Kondo physics
   c) STM spectroscopy with Dirac fermions.

3. Potential applications in engineering:
   a) Detection of gas molecules with great precision
   b) Possibility of nanoscale room temperature transistors.

4. Future:
   a) Controlled sample preparation and better lithography.
   b) More strongly correlated phenomenon such as FQHE.
   c) Graphene based electronics: future direction of nanotechnology?