Interaction of Dirac electrons with spins and point charges

Vacancies in graphene

Vacancy Magnetic moment and Kondo screening

Vacancy Charge and Tunable artificial atom

Twisted bilayer graphene

Eva Y. Andrei

LECTURE NOTES POSTED AT:
http://www.physics.rutgers.edu/~eandrei/links.html#trieste18
Scanning tunneling microscopy and spectroscopy

- Engineering electronic properties
  - Density of states and Landau levels in graphene
  - Scanning tunneling microscopy (STM) and spectroscopy (STS)
  - Defects:
    - Atomic collapse and artificial atom
    - Kondo effect
  - Substrate:
    - Twisted graphene
Kondo Screening of Impurity Moments in Metals

\[ T > T_K \]  
Unscreened

\[ T < T_K \]  
Screened

J antiferromagnetic coupling to electron bath

\[ T_K \propto \exp(-1/\rho J) \]

\[ \rho \text{ density of states at } E_F \]


- Normal metals  
  \[ \rho(E_F) > 0, J > 0 \iff T_K > 0 \]

- Insulators  
  \[ \rho(E_F) = 0 \]
  No Kondo screening

What happens in a pseudogap system?
**Kondo Screening in pseudo-gap systems**

- **Pseudo-gap systems**
  
  \[ \rho(E) \propto E^r \]

  screening suppressed.

  - **\( r = 1 \)** (graphene, high \( T_c \) superconductors)

**\( \mu \approx 0 \) (undoped)**

- Kondo screening only for \( J > J_c \)
- \( J_c \) finite only for asymmetric DOS

**\( |\mu| \gg 0 \) doped**

- Normal Kondo screening

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- C. Cassanello and E. Fradkin, (1996)
- Vojta, Fritz, Bulla EPL (2010)

**Electrical tuning of magnetic moment**
Kondo Screening Experimental Signatures

Resistance minimum

\[ R(T) \]

Magnetization saturation

\[ \chi^1 \rightarrow \chi_{\text{free}} \left[ 1 - \frac{1}{A_T} \right] \]

\( T \)

\[ \times \text{ NO Kondo screening !} \]

Resistance minimum

\[ \times \text{ NO Kondo screening !} \]

Kondo screening

\[ \checkmark \text{ Kondo screening} \]

Measures:

scattering off Kondo cloud

Measures:

Unscreened moment

DOS – Kondo Peak

\[ \text{Kondo Peak at } E_F \]

• Low T linewidth \( \Gamma \)

\[ k_B T_K \sim \Gamma/2 \]

DOS enhancement at \( E_F \)

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Vacancy in graphene

![Graphene image]

- **$V_{\text{g}}=0V$**
- **$\mu=50\text{meV}$**
- **$n=2\times10^{11}\text{cm}^{-2}$**

**Zero mode**

**Kondo**

**$dI/dV$** (a.u.) vs. $V_b$ (V)

**$E_F$**

**DP**
Vacancy Peak

- localized on vacancy site <2nm.
- pinned to the Dirac point
Kondo Temperature

Fit to Fano lineshape

\[
\frac{dI}{dV} = A \left( \frac{\varepsilon + q}{1 + \varepsilon^2} \right)^2 + B
\]

\[
\varepsilon = \frac{E - \varepsilon_0}{\Gamma/2}
\]

\[
k_B T_K \sim \Gamma/2
\]

Fit to T dependence

\[
\Gamma = \sqrt{(\alpha k_B T)^2 + (2k_B T_K)^2}
\]

\[
T_K \approx 70 \text{K}
\]

\[
T_K = 68 \pm 2 \text{K}
\]

\[
\alpha = 6.0 \pm 0.3
\]


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**Gate Dependence**

- **Kondo Peak**
  - Increasing $\mu$

- **Zero mode**
  - Pinned to $E_F$

- **DOS**
  - Zero mode peak

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J. Mao et al
Nature Communications 2018
Reentrant Kondo Screening

Kondo “ON”
-92 meV
-88 meV
-84 meV
-79 meV
-73 meV

Kondo “OFF”
-58 meV
-48 meV
-24 meV
-16 meV
0 meV

Kondo “ON”
10 meV
18 meV
24 meV
30 meV
57 meV

Electrically tuned magnetic moment

J < J_c

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Nature Communications 2018
Model for Kondo screening of vacancy moment

- Anderson impurity model
- Numerical renormalization group calculations

- bare $\sigma$-orbital energy
- On site Coulomb
- Exchange coupling
- Hund coupling
- Critical coupling

Single orbital approximation: 

$$U_{\text{eff}}(\mu) = \begin{cases} 
U_{dd} & \mu \leq 0 \\
U_{dd} + \min(U_{d\pi}, \alpha\mu) & \mu > 0 
\end{cases}$$

References:

Y Jiang et al Nature Communications 2018
What determines $J$?

- $\sigma$ Dangling bond $\leftrightarrow$ localized state $\leftrightarrow 1\mu_B$

$\sigma$ state (in plane) – **orthogonal** to $\pi$ conduction electrons $\leftrightarrow J=0$

- $p_z$ state – **Ferromagnetic** coupling $\leftrightarrow J=0$

$J=0 \leftrightarrow$ NO KONDO SCREENING !!

Haase, P., Fuchs, S., Pruschke, T., Ochoa, H. & Guinea, F. (2011)

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Can $J$ be Finite in Graphene?

- Out of plane distortion of dangling bond
- $\leftrightarrow$ Finite AF coupling with conduction electrons $\leftrightarrow$ Kondo screening

Local Moment Formation and Kondo Effect in Defective Graphene

M. A. Cazalilla, A. Iucci, F. Guinea, and A. H. Castro Neto

Finite Kondo coupling

Corrugated Substrate ??
<table>
<thead>
<tr>
<th>Substrate Corrugation</th>
<th>G/SiO$_2$ 2nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum $T_K$</td>
<td>$T_K \sim 180K$</td>
</tr>
<tr>
<td>% of screened vacancies</td>
<td>Most</td>
</tr>
</tbody>
</table>

Substrate corrugation and Kondo screening

J. Mao et al  
Nature Communications 2018
Substrate corrugation and Kondo screening

<table>
<thead>
<tr>
<th>Substrate Corrugation</th>
<th>G/SiO₂ 2nm</th>
<th>G/G/SiO₂ 1nm</th>
<th>G/hBN 0.2nm</th>
<th>G/G/hBN 0.2nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum $T_K$</td>
<td>$T_K \sim 180K$</td>
<td>$T_K \sim 70K$</td>
<td>No Kondo</td>
<td>No Kondo</td>
</tr>
<tr>
<td>% of screened vacancies</td>
<td>30%</td>
<td>none</td>
<td>none</td>
<td>none</td>
</tr>
</tbody>
</table>

$J$ depends on Local corrugation

$\Rightarrow$ Mechanically controlled magnetism

J. Mao et al. Nature Communications 2018
Global Measurements and Conflicting results

- $R(T) \leftrightarrow$ Kondo screening
  - $T_K$ 20-70K

- $\chi(T) \leftrightarrow$ No Kondo screening
- Moments unscreened at low T

Need Local measurement

Y Jiang et al. Nature Communications 2018

Measures:
- Scattering off Kondo cloud
  - Sensitive to screened Moments only.

Measures:
- Magnetic moments
  - Sensitive to unscreened Moments only.

Global measurements probe complementary properties
Graphene with a twist

- Engineering electronic properties
  - Density of states
  - Landau levels in graphene
  - Scanning tunneling microscopy (STM) and spectroscopy (STS)
  - Atomic collapse and artificial atom
  - Kondo effect
  - Twisted graphene
Twisted graphene – Moire patterns

Twist between layers $\leftrightarrow$ Moiré pattern:

$\theta = 3^0$

Superstructure with period $L$

$L = \frac{a_0}{2\sin(\theta/2)}$

$a_0 \approx 2.46 \text{ Å}$
STM topography: Moiré superstructure


superstructure $L=7.5\text{nm}$

$\theta = 1.79^\circ$

Boundary of area with superstructure
Two peak structure only in twisted region

**Band structure of twisted graphene**

Increasing twist angle $\theta$


- $\theta = 1.16^\circ$
  - $L = 12\, \text{nm}$
  - Sample bias: $85\, \text{mV}$

- $\theta = 1.8^\circ$
  - $L = 7.8\, \text{nm}$
  - Sample bias: $450\, \text{mV}$

- $\theta = 3.5^\circ$
  - $L = 4.0\, \text{nm}$

- $\theta = 20.8^\circ$
  - $L = 0.7\, \text{nm}$
**Band structure engineering with a twist**

J. Lopes dos Santos, A.H. Castro Neto

\[ \Delta K = 2K \sin(\theta/2) \]

\[ \Delta E = \hbar v_F \Delta K \propto \sin(\theta/2) \]
Hybridization

\[ \Delta K = 2K \sin(\theta / 2) \]

\[ \Delta E = \hbar v_f \Delta K - w \]
Van Hove singularities


Hybridization

Twisted graphene develops strong Van Hove singularities
Van Hove singularities


Low energy Band structure and DOS using perturbation theory

\[ \Delta = 90 \text{ meV}, \theta = 1.79^\circ \]
What happens at small twist angles?

Moire units cell contains $1.3 \times 10^4$ atoms!
What happens at small twist angles?

\[ \Delta K = 2K \sin(\theta/2) \]

\[ \Delta E = \hbar v_F \Delta K - w \]

For \( \hbar v_F \Delta K \approx w \) band flattens \( \Rightarrow \) DOS diverges: Van Hove singularities.

Magic angle: \( \hbar v_F K \theta_M \approx w \)

Using \( w \approx 100 \text{meV} \)

\[ \theta_M \approx 1.09^0 \]
For $\theta > 10^0$

low energy band structure of twisted layers is identical to single layer

$$\frac{\tilde{v}_F(\theta)}{v_F} = 1 - 9 \left( \frac{w}{\hbar v_F \Delta K} \right)^2$$

- G.T. Laissardière et al, Nanoletters ASAP (2009)
- Shallcross et al. PRL. 101, 056803 (2008)
Correlation effects

- When the energy scale of electron-electron interactions is comparable to the band-width, correlation effects become important.
- At ½ filling (Fermi energy in middle of gap): Correlated states can emerge: superconductivity, charge density waves, antiferromagnetism, topological insulators etc.

\[ E_{\text{coulomb}} = \frac{e^2}{4\pi\varepsilon_0 \kappa \lambda^2}; \]

\( \lambda \) moire period;
\( \kappa \) dielectric constant
For $\theta = 1.16^0$

- 12meV Gap opens at the Fermi energy!
- Correlation gap – CDW?

- Half Full band – 2 electrons (holes) per moire cell.

- $\frac{1}{2}$ Full band – insulating phase $\approx 4K$
- Insulating phase flanked by 2 superconducting domes slightly off half-filling
- Maximum $T_c \approx 1.7K$
- $T_c/E_F \approx 10^{-1}$ $\leftrightarrow$ strong coupling
- Resembles high Tc superconductors
- BUT tunable doping and $T_c$

$\frac{1}{2}$ Full band – 2 electrons (holes) per moire cell.
**Strongly coupled superconductor**


- ½ Full band – insulating phase ~ 4K
- Insulating phase flanked by 2 superconducting domes
- \( T_c/E_F \sim 10^{-1} \rightarrow \) strong coupling
- Resembles high Tc superconductors
- BUT tunable doping and Tc

**OPEN QUESTIONS:**
- Pairing mechanism
- Gap symmetry
- Nature of insulating phase
Summary of part IV

- Kondo screening in graphene occurs above a critical coupling strength.
- Magnetic moments in graphene can be tuned with gating or local curvature.
- If coupling strength is non-uniform, global measurements are misleading.
- Band structure of bilayer graphene can be tuned with twist angle.
- At small twist angles the DOS develops Van-Hove singularities.
- At the “magic angle” $\theta \sim 1.1^0$ a flat band forms at the charge neutrality point.
- At half filling the flat band develops strong correlations resulting in an insulating phase flanked by superconducting domes.

2D materials are cool!