Dirac Materials
A.V. Balatsky

• New class of materials

• What is the definition of Dirac Materials?

• Similarities and differences between d-wave superconductors, Graphene and Topological Insulators: All are Dirac materials with some common features
• Imaging of k and r space

• Local electronics and spins in graphene and TI

• Gap or no gap in TI?
D. Abergel, A. Black-Schaffer Nordita
H. Dahal - BC
T. Wehling, A. Lichtenstein, K. Scharnberg,
R. Wiesendanger – U Hamburg
M. Katsnelson – U Niemegen
J. Fransson- Uppsala
D. Arovas- UCSD
Z. Huang – UCSD, Los Alamos

Experiment: J.C. Davis group
Y. Zhao, V. Brar, M. Crommie -IETS
L. Mattos, H. Manoharan –Kondo graphene
The Dirac Equation

P. Dirac: “The quantum theory of the electron” (1928)

$i\hbar \partial_t \Psi = (c\vec{a} \cdot \vec{p} + \beta mc^2) \Psi$

with 4x4 Dirac matrices

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \ i = 1, 2, 3; \ \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Describing electrons, protons, quarks, neutrinos...

... with peculiar physical consequences:

- Spin 1/2 and Landé g=2
- Klein paradox and Zitterbewegung
- Antiparticles
- Spin orbit coupling
Dirac materials

• Materials whose low energy electronic properties are a direct consequence of Dirac spectrum $E = v k$: specific heat $\sim T^d$, penetration depth $\sim T$, optical conductivity $\sim T^n$

• How do we “design” Dirac Materials?

• Can be a collective state: 3He superfluid, heavy fermion, organic, high Tc superconductors, density wave states

• Band structure effect – graphene, Topological states, cold atom DM, artificial DM

• Not a Dirac equation (1928)

Dirac materials vs metals

\[ E = v(k - k_F) \]
Defining feature:

**Dimensionality of zero energy states in one less (at least)**
In the Dirac materials. Fewer excitations at low T.
Better control of response and less dissipation.
Important for future energy and device applications.
<table>
<thead>
<tr>
<th>Material</th>
<th>Pseudospin</th>
<th>Energy scale (eV)</th>
<th>References</th>
</tr>
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<tbody>
<tr>
<td>Graphene, Silicene, Germanene</td>
<td>Sublattice</td>
<td>1–3 eV</td>
<td>[5, 6, 17, 19, 36, 37]</td>
</tr>
<tr>
<td>Artificial Graphenes</td>
<td>Sublattice</td>
<td>$10^{-8}$–0.1 eV</td>
<td>[28, 29, 38–40]</td>
</tr>
<tr>
<td>Hexagonal layered heterostructures</td>
<td>Emergent</td>
<td>0.01–0.1 eV</td>
<td>[41–47]</td>
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<tr>
<td>Hofstadter butterfly systems</td>
<td>Emergent</td>
<td>0.01 eV</td>
<td>[46]</td>
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<tr>
<td>Graphene-hBN heterostructures in high magnetic fields</td>
<td></td>
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<tr>
<td>Band inversion interfaces</td>
<td>Spin-orbit ang. mom.</td>
<td>0.3 eV</td>
<td>[48–50]</td>
</tr>
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<td>SnTe/PbTe, CdTe/HgTe, PbTe</td>
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<tr>
<td>2D Topological Insulators</td>
<td>Spin-orbit ang. mom.</td>
<td>$&lt;0.1$eV</td>
<td>[7, 8, 22, 24, 51, 52]</td>
</tr>
<tr>
<td>HgTe/CdTe, InAs/GaSb, Bi bilayer, ...</td>
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<tr>
<td>3D Topological Insulators</td>
<td>Spin-orbit ang. mom.</td>
<td>$\lesssim0.3$eV</td>
<td>[7, 8, 23, 52–55]</td>
</tr>
<tr>
<td>Bi$_{1-x}$Sb$_x$, Bi$_2$Se$_3$, strained HgTe, Heusler alloys, ...</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Topological crystalline insulators</td>
<td>orbital</td>
<td>$\lesssim0.3$eV</td>
<td>[56–59]</td>
</tr>
<tr>
<td>SnTe, Pb$_{1-x}$Sn$_x$Se</td>
<td></td>
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<tr>
<td>$d$-wave cuprate superconductors</td>
<td>Nambu pseudospin</td>
<td>$\lesssim0.05$eV</td>
<td>[60, 61]</td>
</tr>
<tr>
<td>$^3$He</td>
<td>Nambu pseudospin</td>
<td>0.3 $\mu$eV</td>
<td>[2, 3]</td>
</tr>
<tr>
<td>3D Weyl and Dirac semimetals</td>
<td>Energy bands</td>
<td>Unclear</td>
<td>[32–34]</td>
</tr>
<tr>
<td>Cd$_3$As$_2$, Na$_3$Bi</td>
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</tbody>
</table>

Table 1. Table of Dirac materials indicated by material family, pseudospin realization in the Dirac Hamiltonian, and the energy scale for which the Dirac spectrum is present without any other states.
Why Dirac materials: path to control of electronic states

Tunability and control

1. With B, E fields
2. With doping and functionalization
3. With quantum size control: films, ribbons

Bi2Se3

Fe or Sn
R-space vs K-space probes of Dirac Materials

Local probes (r space)
STM, spin imaging with Kerr

Extended probes (k space)
Magnetotransport, thermal conductivity

Theory
Guidance for search of new states
Ab initio, functionalization,
How protected are topological states

T. Hanaguri, A. Kapitulink, H. Manoharan
V. Madhavan, A. Yazdani
S.C. Zhang et al RMP, Nov (2011)
A.C. Neto et al, RMP (2010)

Y. Xia et al.,
Universal response to defects. Why Impurities?

• Why *local* signatures and impurities?
  – *Scientific interests*: applications rely heavily on *functionalization*
  – *Observation* possible by Scanning Tunneling Spectroscopy (STS)
  – *Engineered* electronic states due to imp bands
  – *Microchips at one atom at time approach* ~ 100 impurity atoms/transistor
    mean lifetime pictures will break down.
  – Suggested Quantum Computation operations
    involve *deliberate local perturbations*
Local impurity resonances in d-wave superconductors
d-wave Superconductor: Impurity Resonances

On-site potential
U > 0

On-site LDOS

LDOS Image at \( \Omega \)

Cross shaped state

Impurity states in ANY Dirac point materials

\[ T = \frac{U}{1 - U G(\omega)} \]

\[ G(\omega) = \frac{1}{U} \leftrightarrow \text{small} \]
Impurity states in ANY Dirac point materials
Impurity states in ANY Dirac point materials

\[ \frac{1}{U} = G_i(\omega) \quad \text{new states or resonances} \]
Impurity states in ANY Dirac point materials

\[ \frac{1}{U} = G_i(\omega) \quad \text{or} \quad \text{new states or resonances} \]
Impurity states in ANY Dirac point materials
Local impurity resonances in Dirac Materials: Graphene
Real space signatures I

T. Wehling et. al., PRB 75, 125425 (2007), Peres, A.C Neto, Guinea, Falko

$E_{\text{imp}} = 0.1 \text{eV}$
M.M. Udenga et al., PRL104, 096804 (2010)
Universal response to local defects
Hypothesis: ANY Dirac material has similar resonances

Graphene

D-Wave SC
Local impurity resonances in Topological Insulators, probe of stability

Hanaguri et al, PRB 2010, cond mat 1003.0100
Impurity resonances in Dirac Materials: Topological Insulators, probe of suppressed back scattering


Hanaguri et al, PRB82, 081305(2010);
Resonance as seen in STM


Sassi et al. NATURE COMM | DOI: 10.1038/ncomms6349, (2014)
ARPES on magnetically doped TI and on films

\[ H = \vec{k} \vec{\sigma} + S_z \sigma_z \]

\[ E = \pm \sqrt{k^2 + S_z^2} \]

Fully gapped spectrum

At $B=0$ at Dirac point now there should Be a true gap. The data show finite LDOS.

Gap or no gap for Cr doped sample.
Gap in FM ordered TI seen in STM
Robust conventional IQHE has mobility gaps, not real gaps

Figure 5: Density of states as a function of energy:
   a) of an ideal 2D crystal;
   b) of a 3D crystal or a 2D crystal at lower fields;
   c) of a 2D crystal under higher applied fields.
Gas vs Mobility gap in (A) QHE

Conventional IQHE

Anomalous QHE that does not require a full gap either

\[ \text{Cr}_{0.15}(\text{Bi}_{0.1}\text{Sb}_{0.9})_{1.85}\text{Te}_3 \]

Science 340, 167
Mass acquisition of Dirac fermions in Cr-doped topological insulator Sb$_2$Te$_3$ films

Yeping Jiang, Zhi Li, Cai Li Song, Mu Chen, Richard L. Greene, Ke He, Lili Wang, Xi Chen, Xuewu Ma, and Qi-Kun Xue

Z. Alpichev et al, PRL 108,206102,(2012)

No gap at zero field

Zuoqin Zhang et al. Electrical control of the ferromagnetism in Cr doped Sb$_2$Te$_3$ diluted magnetic topological insulator. to be submitted (2013).
Competing trends due to magnetic scattering

Low energy resonance
- Every impurity (magnetic and nonmagnetic) will produce imp resonances inside Dirac cone = backscattering

Magnetic scattering
- Gap in Dirac spectrum
- Dirac fermion acquire a mass due to spin

\[ H = \bar{k}\vec{\sigma} + S_z \sigma_z \]
\[ E = \pm \sqrt{k^2 + S_z^2} \]

True answer is combination of both effects
Filling of Magnetic Impurity Induced Gap in Topological Insulators by Potential Scattering


FIG. 3: Evolution of the surface local DOS (per energy and area unit)

FIG. 1: Evolution of the band structure as function of the impurity potential $U/M = 0, 1, 2, 3, 4, 5, 6, $ and 10. Other parameters are

Science 329, 659 (2010)

Y. L. Chen, et al.
Artificial Dirac Materials: Nanoscale functionalization in Graphene physics

doi:10.1038/nature10941
Universal response of Dirac materials to local perturbations

Graphene

D-Wave SC

TI
Conclusion

• Dirac materials is a class

• Convergence in multiple materials -> class.

• Defects as test of stability of Topological states

• The future is even more exciting with designed materials coming.

• New imaging to capture exciting new phenomena in quantum materials