Loops of Dirac points in three dimensions

Line of Dirac nodes in hyperhoneycomb lattices

Kieran Mullen, Bruno Uchoa and Daniel T. Glatzhofer, Phys. Rev. Lett. 115, 026403 (2015)

Recommended with a commentary by Rahul Nandkishore, CU Boulder

Introductory courses in solid state physics typically begin with a discussion of (Fermi liquid) metals and band insulators. At zero temperature in d spatial dimensions, the former have a Fermi surface of dimension $d-1$ (and co-dimension [1] 1) where the chemical potential intersects a partially filled band, while the latter have no Fermi surface, with the chemical potential sitting in the band gap. The discovery of Dirac semimetals (of which graphene is probably the earliest and certainly the most famous example) has introduced a qualitatively new possibility. In Dirac semimetals, the conduction and valence bands touch at a discrete set of points, and when the chemical potential is tuned to that point then there arises a zero dimensional Fermi surface with co-dimension d, which in spatial dimensions two and three is clearly intermediate between a metal and a band insulator. This fact, combined with the π Berry phase associated with Dirac points, is responsible for much of the rich phenomenology that has captivated condensed matter physicists over the past decade.

Very recently, it has been realized that in three spatial dimensions there can arise *Dirac line* semimetals, where the conduction and valence bands touch on a line. To my knowledge, this notion was first advanced in [2], albeit in a context where having the line contact at constant energy required considerable fine tuning. The focus of [3] is on a situation where this line contact is naturally non-dispersive (i.e. at constant energy), such that the Fermi surface at perfect compensation consists of a line of Dirac nodes with co-dimension two - a case intermediate between three dimensional Dirac point semimetals and ordinary three dimensional metals. Such 'Dirac line semimetals' provide a qualitatively new playground for solid state physics, of (one may hope) comparable richness to Dirac point semimetals. Specifically, Mullen, Uchoa and Glatzhofer show that in a certain class of three dimensional hyperhoneycomb lattices (Fig.1), a simple tight binding model (without spin orbit interaction) gives rise to a closed loop of Dirac points at zero energy. As pointed out in [2], such a bulk Dirac line node also results in a flat band of surface states. The simplest such

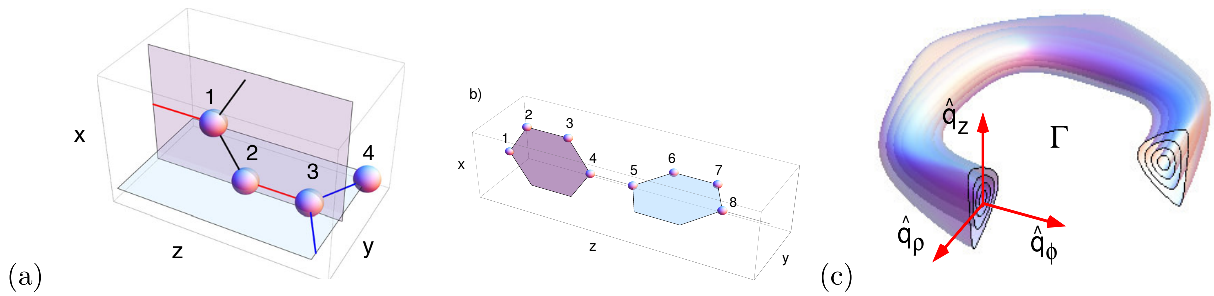

FIG. 1. (a) and (b) show the unit cells of the two simplest hyperhoneycomb lattices that realize Dirac loops in their tight binding dispersion. Subfigure (c) shows the Fermi surface at small but non-zero doping - the Fermi surface is a torus in momentum space which shrinks to a circle as the doping is taken to zero. Figures are taken from [3].

lattice supporting a loop of Dirac nodes is a hyperhoneycomb lattice with a four site unit cell, which the authors argue should be a metastable allotrope of carbon. Such a three dimensional allotrope of carbon, if realized, may then provide a paradigmatic example of a Dirac line semimetal. Alternative material realizations have also been discussed elsewhere. My interest, however, was piqued more by the universal physics that should be associated with such a loop of Dirac points, regardless of the material realization.

The low energy $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for the material discussed in [3] takes the form

$$H(\mathbf{p}) = \sum_{\mathbf{p}} (v_x(\phi)\delta p_x + v_y(\phi)\delta p_y)\sigma_x + v_z(\phi)\delta p_z\sigma_z \tag{1}$$

where σ_x and σ_z are Pauli matrices, the δp_i denote the momentum offset from the closest point on the Dirac loop, the v_i are the Fermi velocities in the corresponding directions, and $0 \leq \phi < 2\pi$ is an azimuthal angle parametrizing position along the loop. Much of the key physics, however, can be exposed by a cylindrically symmetric 'toy model' where the Dirac loop is a circle of radius p_F in the x-y plane. This has a low energy $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian of the form

$$H(\mathbf{p}) = \sum_{\mathbf{p}} v_\perp(p_\perp - p_F)\sigma_x + v_z p_z \sigma_z \tag{2}$$

where $p_\perp = \sqrt{p_x^2 + p_y^2}$. The dispersion takes the form

$$E_\pm(\mathbf{p}) = \pm\sqrt{(v_\perp(p_\perp - p_F))^2 + (v_z p_z)^2} \tag{3}$$

This toy model contains a great deal of physics. At perfect compensation, the Fermi surface is a circle with radius p_F and codimension two, and there is a π Berry phase along any loop that interlocks the Fermi surface. The low energy density of states vanishes linearly with energy - much as in graphene, but now in three dimensions. This too is intermediate between a metal (where the low energy density of states is constant) and a perfectly compensated clean Dirac point semimetal (which in three dimensions has a quadratically vanishing low energy density of states) Meanwhile, on doping away from perfect compensation the Fermi surface turns into a torus.

Dirac loops in three dimensions can support new phenomena not conventionally associated with 3D systems. The authors of [3] highlight this by pointing out one particularly striking new phenomenon: a three dimensional quantized Hall effect in the presence of an constant azimuthal magnetic field. Intuitively, if we consider a single point on the Fermi ring, the Hamiltonian $v_\perp \delta p_\perp \sigma_x + v_z p_z \sigma_z$ looks just like the Hamiltonian for a two dimensional Dirac fermion moving in the $p_\perp - z$ plane, and the application of an azimuthal magnetic field should give rise to a quantized Hall response just as the application of an out of plane magnetic field gives rise to a quantized Hall response for the two dimensional Dirac fermion. More formally, a magnetic field $\mathbf{B} \propto B_\phi \hat{\phi}$ may be represented by a 'Landau gauge' vector potential $\mathbf{A} = -B_\phi \rho \hat{z}$, where $\rho = \sqrt{x^2+y^2}$. Introducing the vector potential into the Hamiltonian through the usual minimal coupling prescription, and squaring the Hamiltonian, Mullen *et al* find that the Hamiltonian can be diagonalized by introducing ladder operators, and the spectrum takes the form

$$E_N = \mathrm{sign}(N)(\sqrt{2 v_\perp v_z}/l_B)\sqrt{|N|} \tag{4}$$

where $l_B \propto 1/\sqrt{B}$ is the usual magnetic length i.e. the spectrum breaks up into a (particle-hole symmetric) tower of Landau levels indexed by integer N, with a 'square root' dependence of energy on magnetic field and on Landau level index, just as in graphene. When the chemical potential lies in the gap between the N^{th} and $(N+1)^{th}$ level, the system has $\sigma_{z\rho} = (2N+1) p_F e^2/h$, allowing for a factor of two coming from spin degeneracy i.e. a radial current induces a voltage bias along the $\hat{z}$ axis, with a quantized proportionality constant that depends linearly on the Fermi radius. Colloquially, an azimuthal magnetic field produces a Hall response in the $\hat{z} - \hat{\rho}$ plane that is like the response of p_F copies of graphene to an out of plane field. This behavior should survive even when the Fermi line is deformed away from a perfect circle, as long as the bulk gaps do not close, and thus may well be observable in Dirac loop materials. Of course, to produce a radially uniform azimuthal magnetic field one would have to apply a time varying electric field $\propto 1/\rho$ along the $\hat{z}$ direction, which experimentally may not be a simple task.

The combination of a Berry phase, a linearly vanishing low energy density of states in three dimensions, and a non-trivial Fermi surface topology provides a qualitatively new playground for condensed matter physics, and there remain many questions still to explore. For example, what are the signatures of Dirac loops in transport, aside from the three dimensional quantum Hall effect discussed above? What is the effect of disorder? Of interactions? Of a combination of the two? What new phases can we access starting from Dirac loop systems and turning on interactions, disorder, and/or external fields? How does the phenomenology differ for Dirac loops and for Weyl loops (without spin degeneracy)? And where and how will this new physics be seen experimentally? While some preliminary steps along these directions have been taken [2, 4, 5], much surely remains to be done. A new chapter has been opened in the study of Dirac materials. There are exciting times ahead.

---

[1] The codimension is the number of directions in which one can move away from the Fermi surface. For a traditional Fermi liquid metal, the codimension is 1 - the direction normal to the Fermi surface. A Dirac point semimetal, however, has co-dimension d, and a Dirac line semimetal has codimension $d-1$. The codimension d_c is important in part because it controls the low energy density of states, which scales as $\nu(E) \sim E^{d_c-1}$ for systems with linear dispersion, and this in turn controls the response functions, the relevance/irrelevance of disorder and interactions, and much besides.

[2] A.A. Burkov, M.D. Hook and L. Balents, *Phys. Rev. B* **84**, 235126 (2011)

[3] K. Mullen, B. Uchoa and D. T. Glatzhofer, *Phys. Rev. Lett.* **115**, 026403 (2015)

[4] Y. Huh, E.-G. Moon and Y. B. Kim, arXiv: 1506.05105

[5] R. Nandkishore, arXiv: 1510.00716