Weyl Semimetals

Mehul Goyal
Arnav Jain
Yashovardhan Rai
Disha Zaveri

The Dirac Equation

In 1928, Paul Dirac Proposed his controversial equation for spin ½ particles which looked like:

$$(i\gamma^{\mu}\partial_{\mu} - m)\Psi = 0$$

It was controversial because it predicted the existence of anti-particles (-ve mass).

However it solved two crucial things :

- **It is of the same order in both space and time**, thereby given equal status to all spatial and temporal dimensions [the Schrodinger equation is second order in space]
- **Equations of motion must be first order in time**, and this equation only uses the the first derivatives with respect to each.

Thus, despite its seeming flaws it achieved a final reconciliation of quantum mechanics and special relativity.

4x4 Gamma matrices and wavefunctions

Dirac's theory makes heavy use of the 4x4 matrices that are called gamma matrices and they follow the following relations:

$$\{\gamma^\mu, \gamma^\nu\} = 0, (\gamma^0)^2 = -(\gamma^i)^2 = I$$

Where i is 1,2....d (in dimensional), these take the form in 3+1 dimensions as:

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \gamma^1 = \begin{pmatrix} 0 & \sigma_1 \\ -\sigma_1 & 0 \end{pmatrix}$$
$$\gamma^2 = \begin{pmatrix} 0 & \sigma_2 \\ -\sigma_2 & 0 \end{pmatrix} \quad \gamma^3 = \begin{pmatrix} 0 & \sigma_3 \\ -\sigma_3 & 0 \end{pmatrix}$$

The wavefunctions are now complex valued vectors, and the two components allow these 'spinors' to naturally allow for 'spin', as opposed to ad-hoc considering 2 wavefunctions

$$\psi^{(+)} = u^{(\phi)}(\vec{p})e^{-ip\cdot x} = \sqrt{\frac{E+m}{2m}}\begin{bmatrix} \phi \\ \frac{\vec{\sigma}\cdot\vec{p}}{E+m}\phi \end{bmatrix} e^{-ip\cdot x} \qquad \psi^{(-)} = v^{(\chi)}(\vec{p})e^{ip\cdot x} = \sqrt{\frac{E+m}{2m}}\begin{bmatrix} \frac{\vec{\sigma}\cdot\vec{p}}{E+m}\chi \\ \chi \end{bmatrix} e^{ip\cdot x}$$

$$\Psi_{total} = \psi^+ \oplus \psi^-$$

We can show various kinds of fermions exist

In 1929, the mathematician Hermann Weyl proposed a simplified version that described **massless fermions** with a definite chirality (or handedness).

In 1937, Ettore Majorana found a modification using real numbers, which described a neutral particle that was its own antiparticle.

It was initially thought that neutrinos would end up being this massless Weyl fermion however with the discovery of a finite neutrino mass meant that no more candidates for a Weyl fundamental particle were left.
Still, within condensed matter we can see possibilities of similar dispersions existing, and in 2015 a group finally found weyl fermions inside crystals.

The Weyl Equation

If in the dirac equation we use m=0, the Up and Down spinor get decoupled and we get a simplified equation of the form:

$$\Sigma \partial_u \gamma^u \Psi = 0$$

Where the summation runs from 0 (representing time) to some odd spatial dimensions (2d+1).

In 1+1 dimensions : $$i\partial_t \Psi = (\gamma^0 \gamma^1 p)\Psi; p = -\partial_x$$

Define a new matrix defined as the product of all gammas :

$$\gamma_5 = \gamma^0 \gamma^1 = \sigma_x$$

Since 'p' happens to be the eigen-value of the hamiltonian as well for m=0 : giving the dispersion relation*

$$i\partial_t \Psi_\pm = \pm p \Psi_\pm \quad E_\pm(p) = \pm p$$

*these are unique from photons as the dirac equation describes half integer spin particles (fermions) and photons are bosons.

The Weyl Equation

If in the Dirac equation we use m=0, the Up and Down spinor get decoupled and we get a simplified equation of the form:

$$\Sigma \partial_u \gamma^u \Psi = 0$$

Where the summation runs from 0 (representing time) to some odd spatial dimensions (2d+1)

$$\gamma_5 = i^k \Pi \gamma^\mu$$

In 1+3 dimensions :

$$i\partial_t \Psi_\pm = H_\pm \Psi_\pm$$

Similar procedures give us:

$$H_\pm = \mp \vec{p}.\vec{\sigma}$$

Symmetries

There are two symmetries important to us here: Inversion (P) and Time Reversal (T)

Inversion: $H(-\mathbf{k}) = PH(\mathbf{k})P^{-1}$ $E_{n,s}(-\mathbf{k}) = E_{n,s}(\mathbf{k})$

Time Reversal: $H(-\mathbf{k}) = TH(\mathbf{k})T^{-1}$ $E_{n,-s}(-\mathbf{k}) = E_{n,s}(\mathbf{k})$

PT symmetry: $E_{n,-s}(\mathbf{k}) = E_{n,s}(\mathbf{k})$

Hence when Hamiltonian is PT symmetric, it is doubly degenerate;

If Hamiltonian is only P symmetric, bands are typically non degenerate.

When Hamiltonian is only T symmetric, it is degenerate only at Time Reversal Invariant Momenta (TRIM).

This is called **Kramer's degeneracy**. (Ref 4 for a complete discussion and proof)

Accidental Degeneracies

In general, upto a constant shift, the hamiltonian at any point can be represented as :

$$H(\mathbf{k}) = f_0(\mathbf{k})\mathrm{I} + f_1(\mathbf{k})\sigma_x + f_2(\mathbf{k})\sigma_y + f_3(\mathbf{k})\sigma_z$$

The difference in energy eigenvalues =

$$\Delta E = 2\sqrt{f_1^2 + f_2^2 + f_3^2}$$

In the absence of any symmetry, all three functions have to independently be zero for the band gap to be zero.

However if we have certain symmetries, we can find the degenerate points by solving for the points where the constrained set of functions are zero simultaneously

For example, time reversal symmetry requires f2=0 everywhere, f1 and f3 can be solved for.

$$\psi(r,t) = e^{-i\hbar Ht}\psi(r,0)$$
$$T\psi(r,t) = \psi(r,-t) = \psi^*(r,t)$$

Thus imaginary part of hamiltonian must be zero in this case

Time Reversal Invariant Momenta

Kramer's degeneracy says that if there is Time reversal symmetry in a system

(Eg : no magnetic field is applied),

then there are is a degenerate partner state for every energy eigenfunction.

$$\mathcal{H}\Psi = E\Psi \quad \& \quad HT\Psi = ET\Psi$$

In the context of crystal structure, TRIM refers to points in the brillouin zone that when Time reversal is applied, become equivalent to the negative momentum states, upto a reciprocal lattice vector.

They will end up having the same energy and the other state has the opposite spin.

$$T\Psi_s(k,t) = \Psi_{-s}(-k + G = k, -t)$$

In 1D, Edges of the brillouin zone are TRIMS, in a 2D square lattice, Centre of the sides of the FBZ are trim. The zero momentum state is a trivial example of a TRIM.

This is a relatively easy way to find degenerate states, but generally we will look for systems where the band touching point is near the fermi level.

What are we looking for:

Remember, the effective Hamiltonian for a 2 level system is

$$H(\mathbf{k}) = f_0(\mathbf{k})\mathrm{I} + f_1(\mathbf{k})\sigma_x + f_2(\mathbf{k})\sigma_y + f_3(\mathbf{k})\sigma_z$$

Around a point of band touching, The hamiltonian can be expanded as :

$$H(k) \sim f_0(k_0)I_3 + v_0\delta k I_3 + \Sigma v_a \delta k \sigma^a$$

$$v_\mu = \nabla_k f_\mu(k)\|_{k=k_0}$$

Dirac Cones!

https://www.desmos.com/calculator/8cds0v3mc4

- Shifting Term($f_0(k_0)$): Moves the dirac cone up or down. In practical terms, it decides whether the material behaves as a conductor or insulator
- Tilt Term(v_0): This term causes an asymmetry in the Dirac cone, tilting it in a specific direction. This tilt can create an "overtilted" cone if it becomes too strong. In overtilted cone, electrons and holes co-exist at all energies near dirac point
- Widening Term (v_a): Controls the steepness of the dirac cone. The steeper the dirac cone, higher the group velocity near the node.

Chern Number

We have a 2x2 Hamiltonian of the form $H = \pm \vec{p}.\vec{\sigma}$. We can write the eigenvectors as

$$|-\rangle = \begin{pmatrix} sin\frac{\theta}{2} \\ -e^{i\phi}cos\frac{\theta}{2} \end{pmatrix} \quad |+\rangle = \begin{pmatrix} cos\frac{\theta}{2} \\ e^{i\phi}sin\frac{\theta}{2} \end{pmatrix}$$

Consider the $|+\rangle$ state . We can now compute the Berry connection $\langle + | i\nabla_{\theta,\phi} | + \rangle$

We get $A_\theta = 0$ and $A_\phi = -\frac{sin^2\frac{\theta}{2}}{rsin\theta}$. We can now compute the Berry curvature $\nabla \times A$

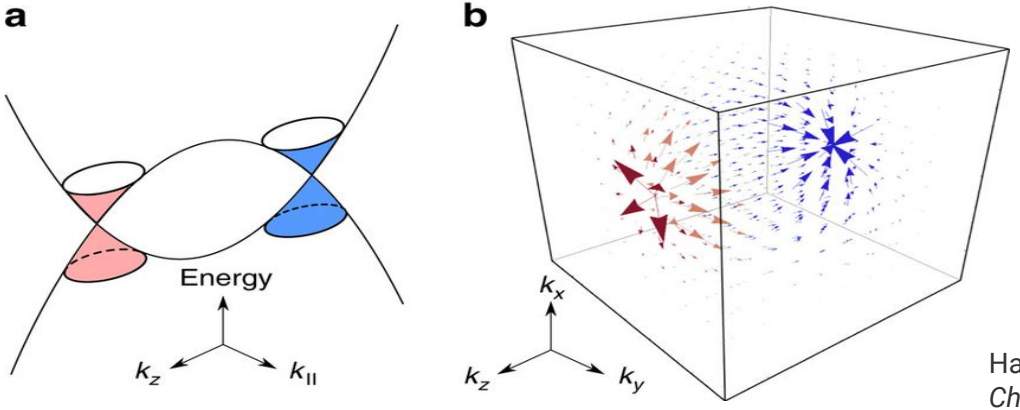
We get Berry curvature $\Omega_r = \frac{1}{r\sin\theta}[\partial_\theta(A_\phi \sin\theta) - \partial_\phi \mathcal{A}_\theta]\hat{r} = -\frac{1}{2r^2}\hat{r}$

Integrating over a spherical surface close to the node, we get $\int_{\text{sphere}} \frac{1}{2r^2}\hat{r} \cdot d\mathbf{S} = 2\pi(-1)$

We get a Chern Number of -1 . Similarly, from here we see can also get Chern Number of +1 for $|-\rangle$

Weyl nodes are sources of Berry flux!

- Berry curvature acts like a magnetic field in the parameter space. In this analogy, the Weyl nodes behave as monopole-like sources for Berry flux. A node with positive chirality acts as a “source” while a node with negative chirality acts as “sink”.
- According to the Nielsen-Ninomiya Theorem (we won’t go into details of it), Weyl nodes must come in pairs of opposite chirality within the Brillouin zone. This ensures that the total Berry flux (monopole charge) sums to zero over the entire momentum space.
- A heuristic way to understand it is through periodicity of the Brillouin zone.



Hao-Nan Cui *et al* 2023
Chinese Phys. B 32 077305

Model Hamiltonian

A model Hamiltonian was proposed by Koshino and Hizbullah, 2016:

$$H = v\tau_x(\sigma \cdot \mathbf{k}) + m\tau_z + b\sigma_z + b'\tau_z\sigma_x = \begin{pmatrix} m\mathrm{I} + b\sigma_z + b'\sigma_x & v\sigma \cdot \mathbf{k} \\ v\sigma \cdot \mathbf{k} & -m\mathrm{I} + b\sigma_z - b'\sigma_x \end{pmatrix}$$

The eigenvalues of this Hamiltonian are for b' = 0:

$$\epsilon_{su}(k) = s\sqrt{m^2 + b^2 + v^2k^2 + \mu 2b\sqrt{v^2k_z^2 + m^2}} \quad \mu = \pm 1 \quad \text{and} \quad s = \pm 1$$

Point nodes are $k = (0, 0, \pm\frac{\sqrt{b^2 - m^2}}{v})$

The eigenvalues with m = b = 0 are:

$$\epsilon_{su}(k) = s\sqrt{v^2k_x^2 + [v\sqrt{k_y^2 + k_z^2} + \mu b']^2}$$

Zero energy contour: $k_x = 0$ and $\sqrt{k_y^2 + k_z^2} = \frac{b'}{v}$

Energy Spectra for Hamiltonian

|m|>|b|, b' = 0

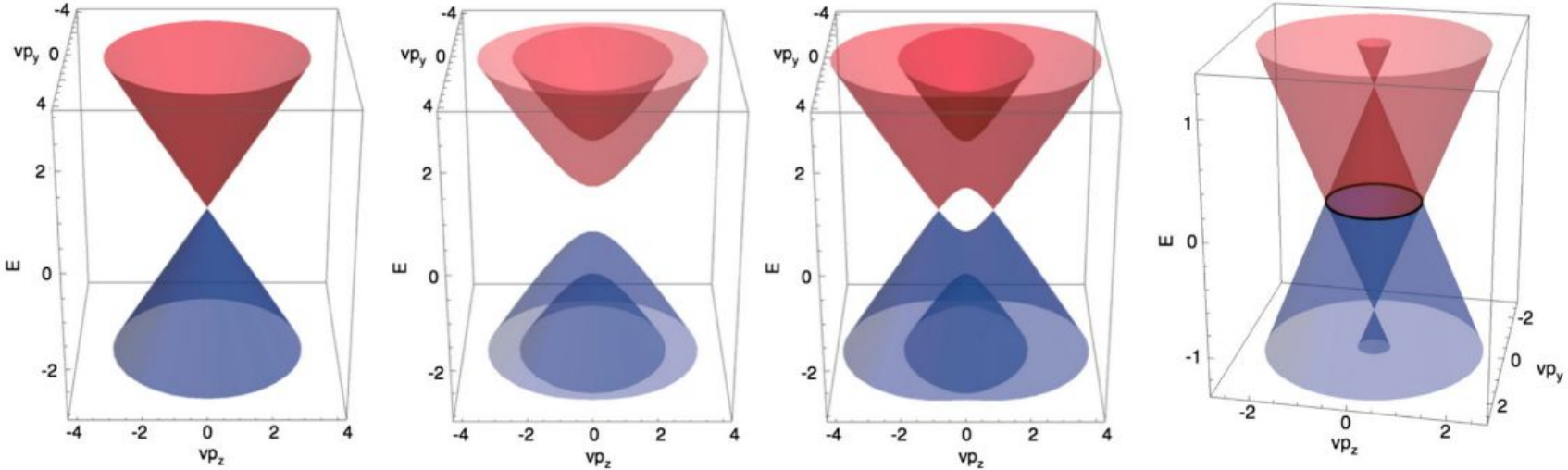
|m|<|b|, b' = 0

m = b = b' = 0

m = 1, b = 0.5, b' = 0

m = 0.5, b = 1, b' = 0

m = b = 0, b' = 1



Dirac semimetal

magnetic semiconductor

Weyl semimetal

Line node

https://www.desmos.com/3d/ycbhxelsja

TI Multilayer Heterostructure

The multilayer is a bulk 3D TI when $\Delta_D > \Delta_S$ and a normal insulator for $\Delta_D < \Delta_S$.

$$\mathcal{H}(\mathbf{k}) = v_F k_y \sigma^x - v_F k_x \sigma^y + m_\pm(k_z)\sigma^z, \qquad (14)$$

where $m_\pm(k_z) = b \pm \Delta(k_z)$, b is the coefficient of the b^z term (magnitude of the spin slitting), and

$$\Delta(k_z) = \sqrt{\Delta_S^2 + \Delta_D^2 + 2\Delta_S\Delta_D \cos(k_z d)}. \qquad (15)$$

Weyl Nodes are found at:

$$k_z^\pm = \frac{\pi}{d} \pm \frac{1}{d} cos^{-1}\left(\frac{\Delta_S^2+\Delta_D^2-b^2}{2\Delta_S\Delta_D}\right)$$

The Weyl nodes move through the BZ and can annihilate at the BZ edge for a critical value of b giving a fully magnetized state

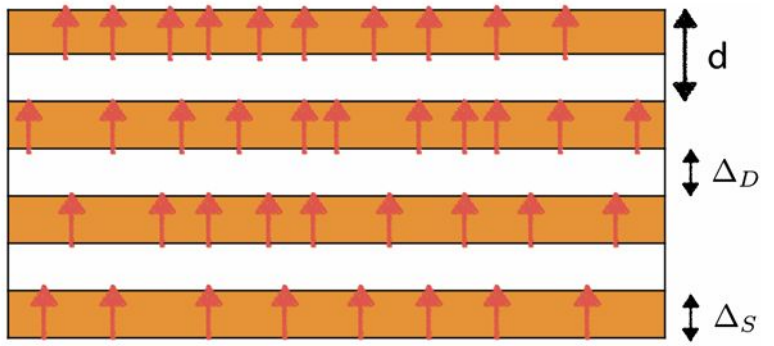


FIG. 4. A heterostructure model of a Weyl semimetal of topological and normal insulators. Doped magnetic impurities are shown by arrows. d is the real space periodicity of the lattice. Δ_S and Δ_D are tunneling between topological surface states on the same topological insulator layer and between different layers, respectively. From Burkov, 2015a.

Symmetries: TRS Broken

Simplest WSM: assume inversion with TRS broken.

Consider the following magnetically ordered cubic system with two orbitals per site:

$$H(\mathbf{k}) = t_z(2 - \cos k_x a - \cos k_y a + \gamma - \cos k_z a)\tau_z + t_x(\sin k_x a)\tau_x + t_y(\sin k_y a)\tau_y.$$

$$H(\mathbf{k}) \to \tau^z H(-\mathbf{k})\tau_z$$

Solution: Weyl nodes at $\cos k_0 = \gamma$ for $-1 < \gamma < 1$ $\pm\mathbf{k}_0 = (0, 0, \pm k_0)$

Going from $\gamma = -1$ to 1 results in Weyl nodes coming from BZ boundary to the centre and annihilating each other!

Symmetries:Parity Broken

Total number of Weyl points must be 4-fold

Visualised as transition between a 3D TI and trivial insulator

In presence of inversion: fourfold degeneracy at TRIM leads to Dirac dispersion and transition proceeds via a Dirac point. Tune only one parameter.

Breaking inversion: Tune additional crystal momenta to move Weyl nodes towards each other and annihilate them.

Tilt of the Weyl Cone

Recall
$H(k) \sim f_0(k_0) I_3 + v_0 \delta k I_3 + \Sigma v_a \delta k \sigma^a$
We had taken $v_0 = 0$ as it is forbidden by Lorentz symmetry in vacuum. It can appear in a linearized long wavelength theory near an isolated twofold band crossing in a crystal.

Sufficiently large v_0 produces a new momentum space geometry with open constant energy surfaces- type II WSM

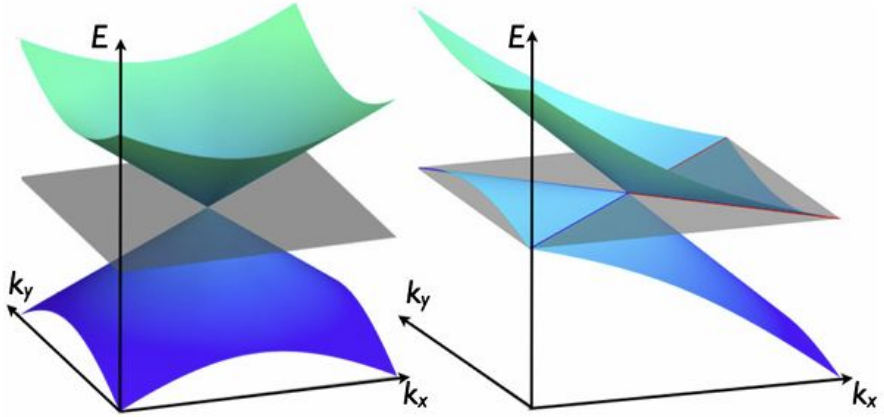


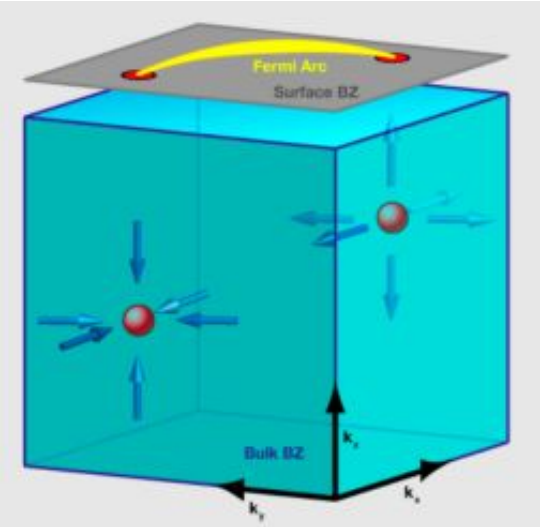
FIG. 5. (Left) Conventional type I Weyl point with pointlike Fermi surface. (Right) Type II Weyl point is the touching point between electron and hole pockets. Red and blue (highlighted) isoenergy contours denote the Fermi surface coming from electron and hole pockets with chemical potential tuned to the touching point.

Fermi Arcs

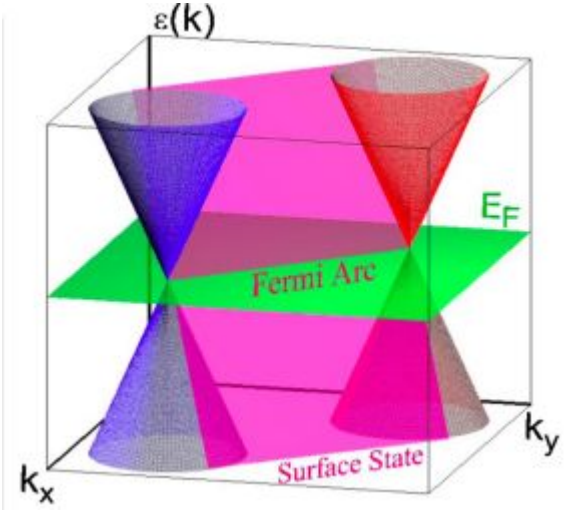
Surface states are generally found in the bulk band gap. However in a WSM, the band is gapless. However there exist surface states due to the chirality of the Weyl points.

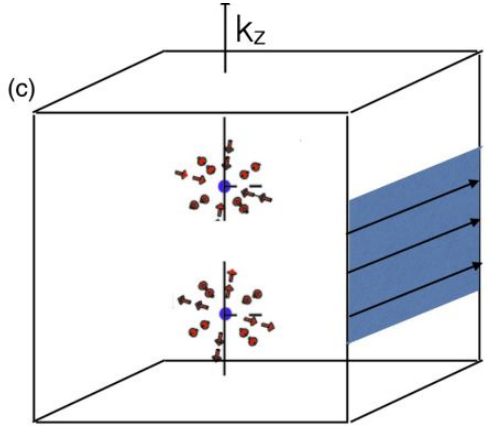
To define, we label surface states with a crystal momenta of the 2D surface BZ (sBZ).

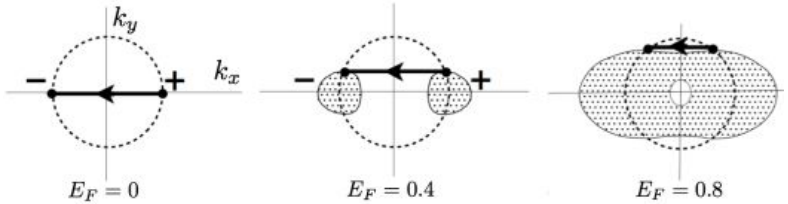
We can define the surface states at all points of the sBZ, except the projection of the Weyl points onto the sBZ



On taking the Fermi level away from the nodes, the projection onto the sBZ is a pair of filled disks enclosing the Weyl node momenta.







Appendix A: Desmos Plots

Model Hamiltonian: https://www.desmos.com/3d/od4dbtk4h1

Dirac cone: https://www.desmos.com/calculator/njzfx7y3cr

Mathematica

References

1) Weyl and Dirac semimetals in three dimensional solids: NP Armitage, EJ Mele and A Vishwanath, Rev. Mod. Phys. **90**, 015001
2) Three Lectures on Topological Physics of Matter: E Witten, https://arxiv.org/pdf/1510.07698
3) Weyl Metals: AA Burkov, Annual Rev of Cond Mat Phys, Vol 9, 2018
4) Lecture Notes, Phys 221A, Robert G Littlejohn, Fall 2019 https://bohr.physics.berkeley.edu/classes/221/1112/notes/timerev.pdf
5) Topological nodal semimetals : A. A. Burkov M. D. Hook and Leon Balents, PHYSICAL REVIEWB 84, 235126 (2011)
6) Koshino, M., and I.F. Hizbullah, 2016, Phys. Rev. B 93, 045201.