Irradiated three-dimensional Luttinger semimetal: A factory for engineering Weyl semimetals

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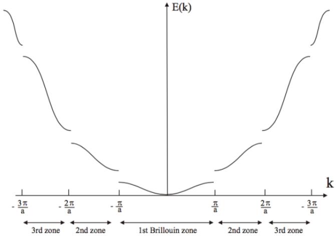
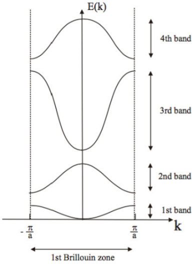
Contents

Band Structure

- Mathematical representation of all occupied and unoccupied energy levels in the lattice of a crystal
- Indispensable apparatus in study of properties of a crystalline solid
- Two types of bands: Valence and Conduction band



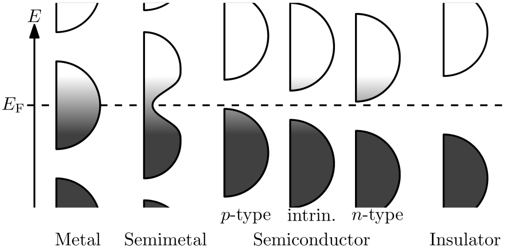


[1]

[1] Solid State Physics - University of Cambridge Part II Mathematical Tripos by David Tong

Classification of Solids

- Classification the basis of gap between valence and conduction band
- 4 types of solids: Metal, semimetal, semiconductors and insulators



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[2] Wikipedia

Topology

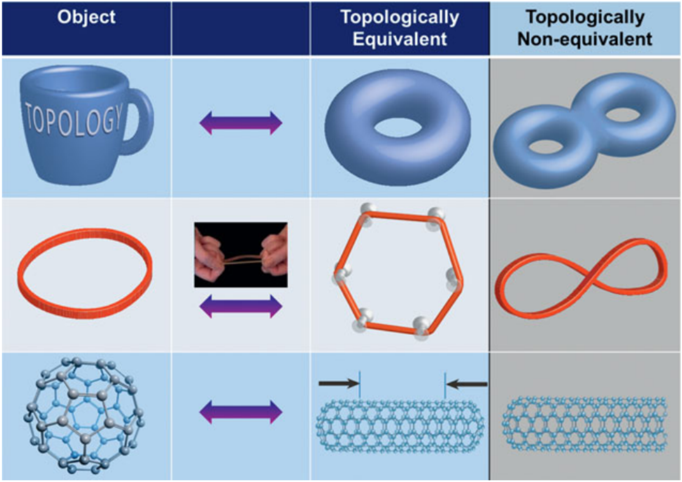
- Properties of spaces that are invariant under continuous deformations
- Genus(g) - Simply, number of holes present on the surface
- **Gauss-Bonet Theorem:**

$$\int_S \kappa dA = 4\pi(1-g)$$

[3]

[3] Wikipedia

Some Illustrations



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[4] A topological twist on materials science by Sanju Gupta and Avadh Saxena

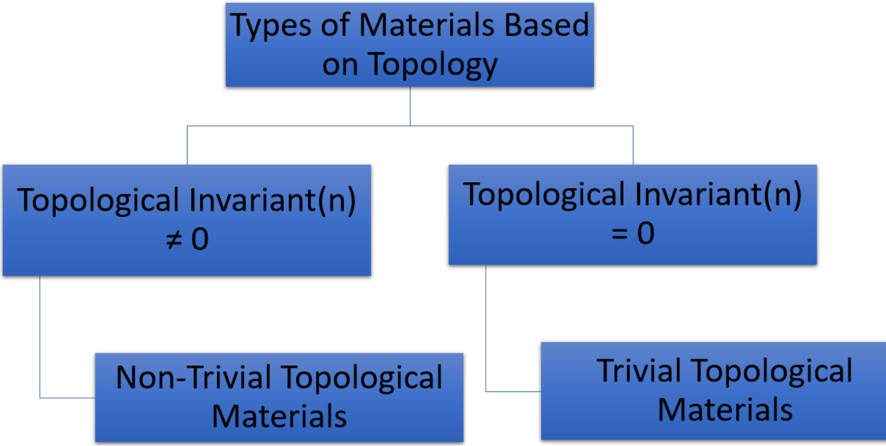
Connection of Topology to Band Structure

Is there any other way to classify solids ?

Yes by Topology of Band Structures

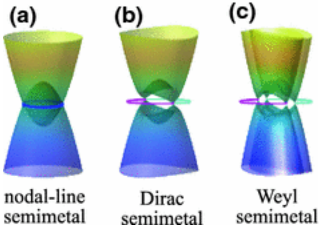
How?

Presence of Topological Invariants


Types of Materials Based on Topology
Topological Invariant(n) ≠ 0
Topological Invariant(n) = 0
Non-Trivial Topological Materials
Trivial Topological Materials

Topological Semimetals

- Topologically nontrivial gapless materials where the conduction and the valence bands cross in the Brillouin zone and the crossing cannot be removed by perturbations preserving concerned crystalline symmetries
- Protected band crossings are present near the Fermi energy and exhibit nonzero topological charges
- The topological charges are basically integer invariants calculated around lines or spheres surrounding the nodes



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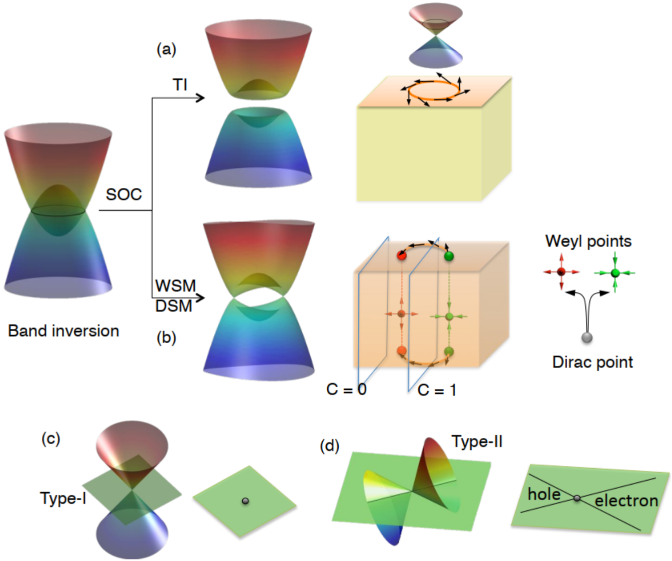
[5] Momentum and Real-Space Study of Topological Semimetals and Topological Defects by Haim Beidenkopf

Weyl Semimetal

- Semimetals whose low-energy excitation are the Weyl fermions
- Weyl fermions are massless particles proposed by Hermann Weyl in 1929 but discovered very recently in condensed matter systems
- Bands dispersion of Weyl semimetal is linear in 3D momentum space through a node known as Weyl point
- The Berry curvature becomes singular at Weyl points that act as monopoles in the momentum space with a fixed chirality, i.e. ,a source ("+" chirality) or a sink ("-" chirality)
- Weyl points always appear in pairs to avoid the divergence of Berry flux
- The total Berry phase in the 2D k plane between a pair of Weyl points gives nonzero Chern number while it is zero for other 2D planes



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[6] Topological Materials: Weyl Semimetals by Binghai Yan and Claudia Felser

Types of Weyl Semimetals

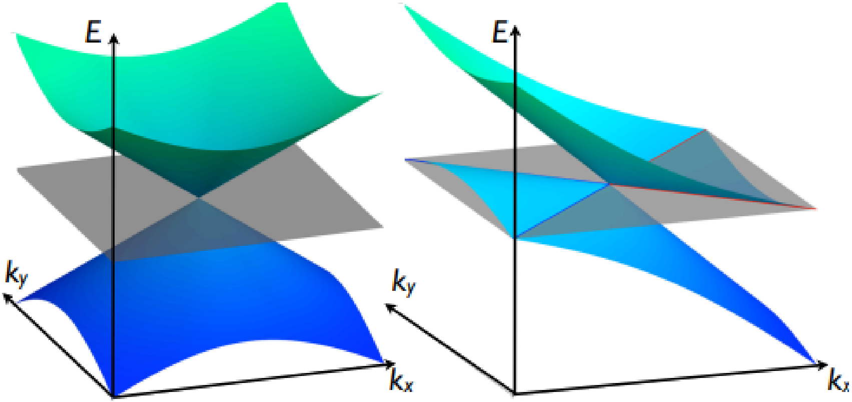

Figure: Type I(left) and Type II(right) Weyl Semimetal

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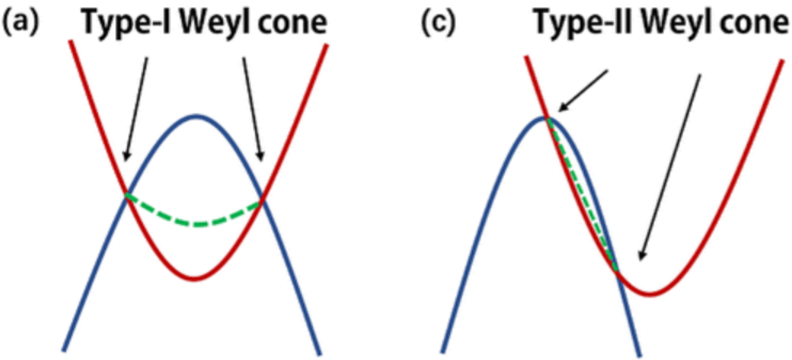
[7] Type II Weyl Semimetals by Alexey A. Soluyanov et al

Types OF Weyl Nodes



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[8] Quasiparticle interference on type-I and type-II Weyl semimetal surfaces: A review by Hao Zheng and M. Zahid Hasan

Using Bloch wavefunctiion in the Schrodinger's equation we get:

$$[\frac{\hbar^2 k^2}{2m} + \frac{\hbar}{m}\vec{k}\vec{p} + \frac{P^2}{2m} + V(r)]u_{n,k}(r) = E_n u_{n,k}(r)$$

The k.p term can be taken as the perturbation to the gross Hamiltonian to get the description of heavy and light holes, given by:

$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{m^2 k^2} \sum_{m \neq n} \frac{\langle u_{n,0}|K.p|u_{m,0}\rangle}{E_{n0} - E_{m0}}$$

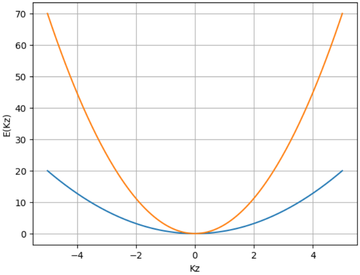
Luttinger-Kohn Hamiltonian describes a system with doubly degenerate 4-band structure. Spin orbit coupling breaks the sixfold degenerate $P_{3/2}$ and $P_{1/2}$ valence orbitals into 4 high energy and 2 low energy bands, and with further K.P perturbation, the 4 fold degeneracy is lifted to give heavy and light hole bands.

Using group theory and representation theory, one can derive the Luttinger-Kohn Hamiltonian given by:

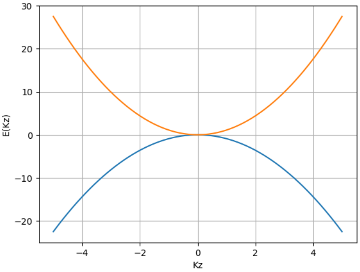
$$H_{LK} = \frac{1}{2}\int_{\mathbf{k}} c^{\dagger}(\mathbf{k})\left(\left(\lambda_1 + \frac{5}{2}\lambda_2\right)k^2 - 2\lambda_2(\mathbf{J}.\mathbf{k})^2 - \mu\right)c(\mathbf{k})$$

where α and β are phases and J are spin 3/2 operators.

- The Luttinger-Kohn Hamiltonian incorporates a quadratic band touching, includes spin orbit coupling and relativistic effects which describes the semi metal physics. For our case, the spin orbit coupling and relativistic terms are ignored.
- λ_1, λ_2 are related to the mass of the light and heavy hole in the band structure.
- The bands are doubly degenerate and show bending depending on λ_i values.



$\lambda_1 = 0.1,\ \lambda_2 = 0.5$



$\lambda_1 = 0.1,\ \lambda_2 = 0.5$

Floquet Theory

- **Floquet Theorem:** Solutions of a periodic linear differential equation:

$$\frac{\partial \vec{x}}{\partial \vec{t}} = X(t+T) \forall X(t+T) = X(t)$$

given by:

$$\vec{x} = exp(-i\alpha t)\vec{y}(t)$$

where $\vec{y}(t+T) = \vec{y}(t)$

- For a time periodic Hamiltonian, i.e., $H(t) = H(t+T)$, Floquet-Schrodinger equation is given by:

$$(H(x,t) - i\hbar\frac{\partial}{\partial t})|\Psi(x,t)\rangle = 0$$

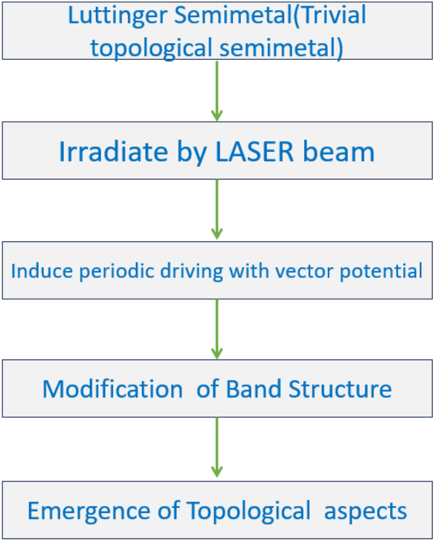
where $H(x,t) = H_0(x) + V(x,t)$, $V(x,t) = V(x,t+T)$, T is time period of Hamiltonian

- Unitary operator:
  $U(T) = \mathcal{T} exp[-i \int_0^T H(t)dt] = exp[-iH_F T]$, where $\mathcal{T}$ is time ordering operator
- $\hat{U}(t_0 + T, t_0)|\Psi_\alpha(t_0)\rangle = exp(-i\epsilon_n T/\hbar)|\Psi_\alpha(t_0)\rangle$
- $exp(\frac{-i}{\hbar} T \hat{H}^F_{t_0}) = \hat{U}(t_0 + T, t_0), \hat{H}^F_{t_0}|u_n(t_0)\rangle = \epsilon_n|u_n(t_0)\rangle$
- $H_{eff} = H_F = \frac{i}{T} Log(U)$
- Eigenvalues of H_F are ϵ_α, diagonalizing $\hat{U}(t_0 + T, t_0)$
- $\hat{H}^F_{t_0}$, acts as $\hat{H}_{eff}$, if observation is stroboscopic, i.e., $t_0, t_0 + T, t_0 + 2T, ..., t_0 + nT$
- $H(\mathbf{k}, t) = \Sigma_m H_m(\mathbf{k}) exp(im\omega t)$
- $\hat{H}_{\pm m}(\mathbf{k}) = \frac{1}{T} \int_0^T dt exp(\pm im\omega t)\hat{H}(k, t)$, $\hat{H_m} = \hat{H_{-m}}^\dagger$

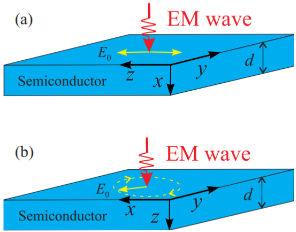
Floquet Perturbation Theory

- In real systems the Hamiltonian is not time periodic when unperturbed
- Add a time periodic perturbation/drive to the systems(say a sinusoidal vector potential).
- Using different approaches like Floquet-Magnus expansion, degenerate perturbation and other methods to calculate the required parameters
- Different results for different regimes of frequency like high frequency and low frequency regime
- In high frequency regime the effective Hamiltonian: $H_{eff}(\mathbf{k}) = H_0 + \sum_{n\geq 1} \frac{[H_{+n}, H_{-n}]}{n\omega} + O(\frac{1}{\omega^2})$ where H_0 is unperturbed Hamiltonian

Formalism to Study Irradiation of Luttinger Semimetals



- Periodic driving is induced by laser light with a vector potential $A(t) = (A_x cos(\omega t), A_y \eta sin(\omega t), 0)$, where η - handedness of polarization
- $H(\mathbf{k}, t) \rightarrow H(\mathbf{k} - e\mathbf{A}/\hbar, t)$
- $H_{eff}(k) = H_0(k) + \frac{[H_1, H_{-1}]}{\omega} + \frac{[H_2, H_{-2}]}{2\omega}$
- $H_1 = (\lambda_1 + \frac{5}{2}\lambda_2)\mathbf{k}.\mathbf{A} - 2\lambda_2\{\mathbf{J}.\mathbf{k}, \mathbf{J}.\mathbf{A}\}$,
  $H_2 = \frac{1}{4}[(\lambda_1 + \frac{5}{2}\lambda_2)\mathbf{A}^2 - 2\lambda_2(\mathbf{J}.\mathbf{A})^2]$
- Floquet perturbation series controlled by $\gamma = \lambda e^2 E^2/\hbar\omega^3$, where $\lambda = \lambda_1 or \lambda_2$.



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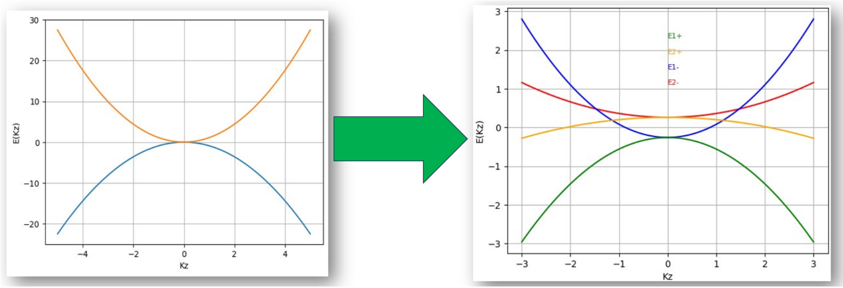
[9] Floquet engineering of the Luttinger Hamiltonian by O. V. Kibis et al

Effect of Circularly Polarized Light

- Here, LSM is irradiated by off-resonant circularly polarized light where $A_x = A_y = A$
- Rotational symmetry ensures appearance of Weyl points appear on only k_z axis. so taking $k_x = k_y = 0$ we get:
  $H_{eff}(k_z) = H_0(k_z) + \frac{2i\eta A^2\lambda_2^2}{\omega}(-k_z^2[\{J_x, J_z\}, \{J_y, J_z\}]$
  $+\frac{A^2}{8}[J_y^2 - J_x^2, \{J_x, J_y\}])$
- $E_{1,\pm} = (\lambda_1 + 2\lambda_2)k_z^2 \pm [3A^2\lambda_2^2\eta(A^2 - 8k_z^2)]/2\omega - \mu$
  $E_{2,\pm} = (\lambda_1 - 2\lambda_2)k_z^2 \pm [3A^2\lambda_2^2\eta(A^2 + 8k_z^2)]/2\omega - \mu$
- In $H_{eff}(k_z)$ time reversal symmetry is broken but inversion symmetry is present
- Double degeneracy is lifted and four non degenerate bands appear which intersect in pairs to give rise to Weyl nodes at $\vec{K_1} = (0, 0, \pm A/2\sqrt{2})$ and $\vec{K_2} = (0, 0, \mp A^2\sqrt{3\lambda_2/\omega})/2$



- $W_n = \frac{1}{8\pi}\int_S d^2k\epsilon^{ijk}\mathbf{n}.(\partial_j\mathbf{n}\times\partial_k\mathbf{n})$ where $\mathbf{n}$ is a unit vector
- $W_n(K_1) = \pm 1,\ W_n(K_2) = \pm 2 \implies$ single and double-Weyl nodes co-exist at different energies
- At point $A_m = \pm\sqrt{\omega/6\lambda_2}$ two types of nodes merge to form triply degenerate point(TDP) .

Evolution of Luttinger Semimetal to Weyl Semimetal(Bands Bending Opposite Way)

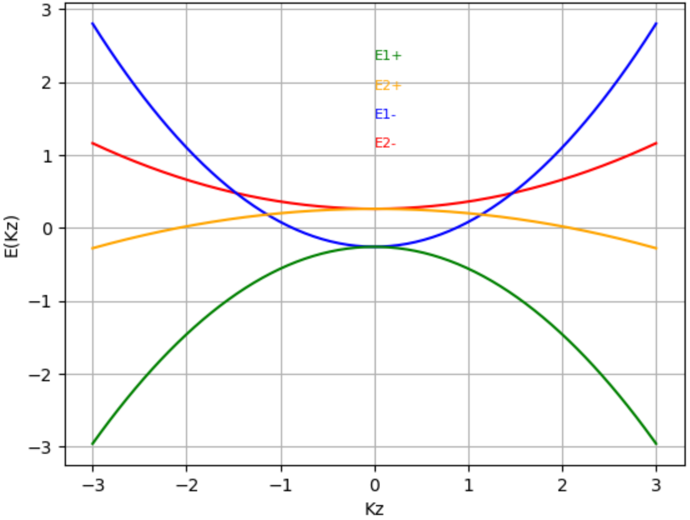


Figure: A=2,λ_1=0.1,λ_2=0.5,ω=20, μ=0 η=1

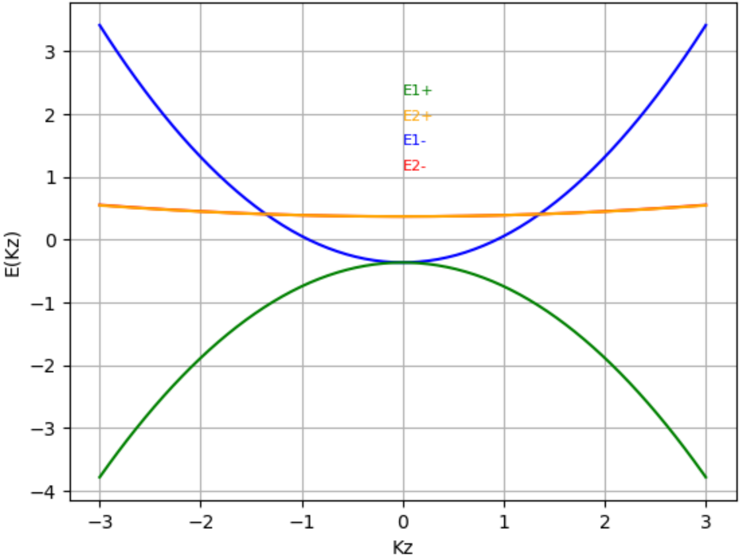


Figure: A=2.58,λ_1=0.1,λ_2=0.5,ω=20, μ=0,η=1

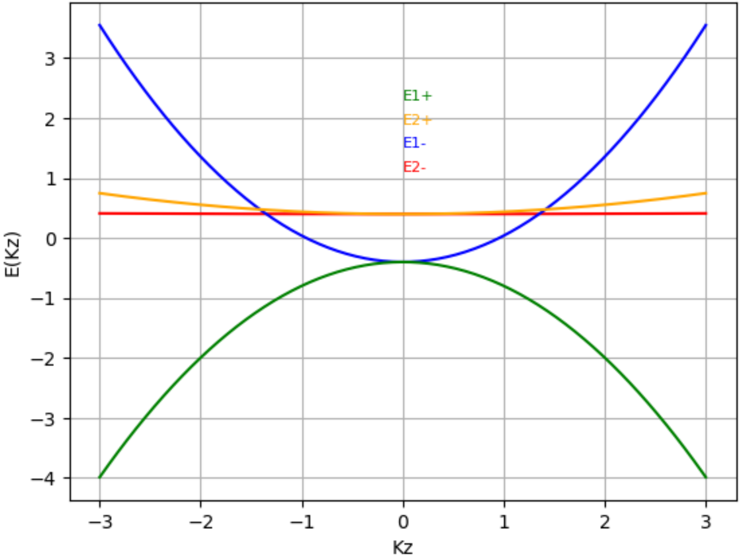


Figure: A=2.7,λ_1=0.1,λ_2=0.5,ω=20, μ=0 η=1

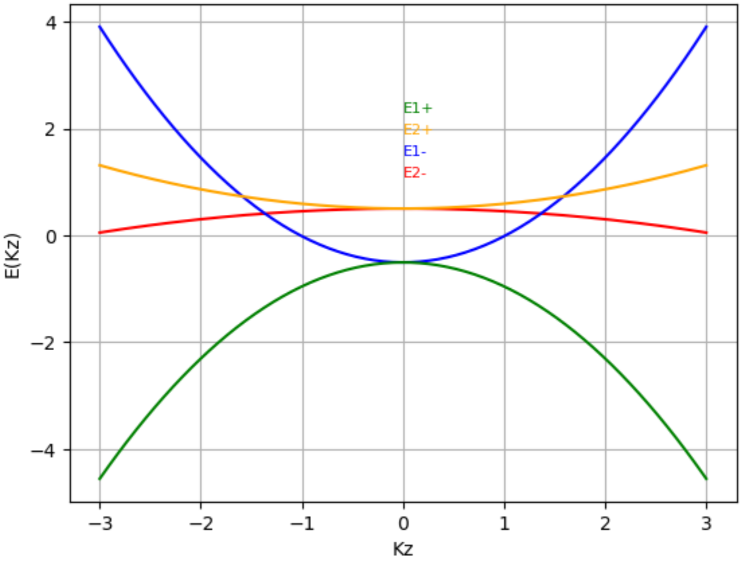


Figure: A=3,λ_1=0.1,λ_2=0.5,ω=20, μ=0 η=1

Evolution of Luttinger Semimetal to Weyl Semimetal(Bands Bending Same Way)

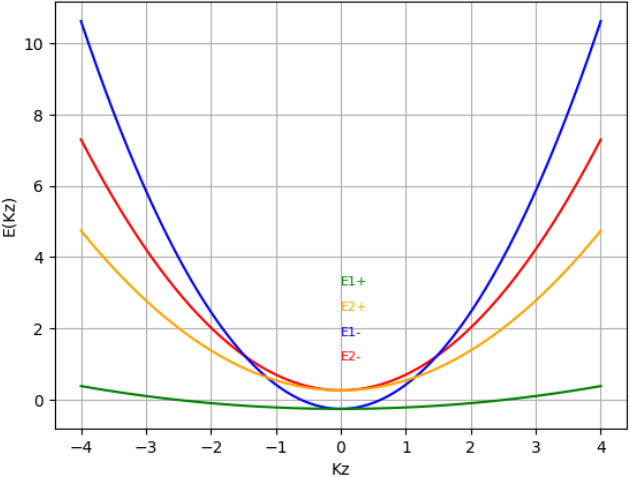


Figure: A=2,λ_1=1.8,λ_2=0.5,ω=20, μ=0 η=1

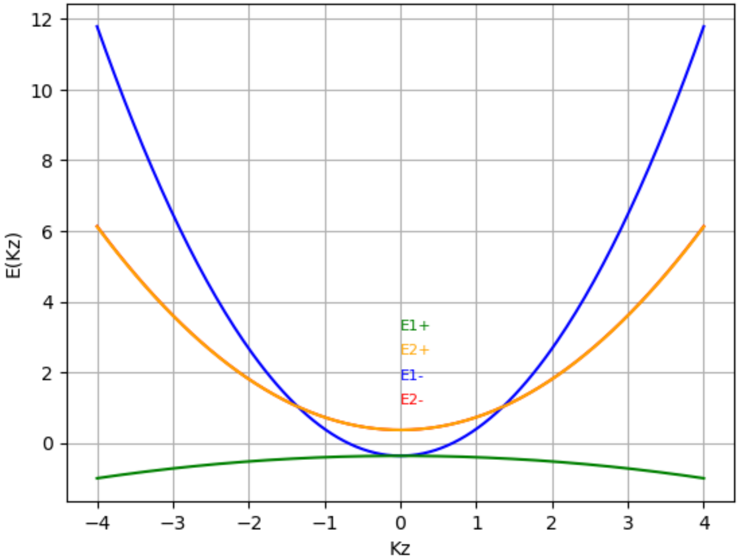


Figure: A=2.58,λ_1=1.8,λ_2=0.5,ω=20, μ=0 η=1

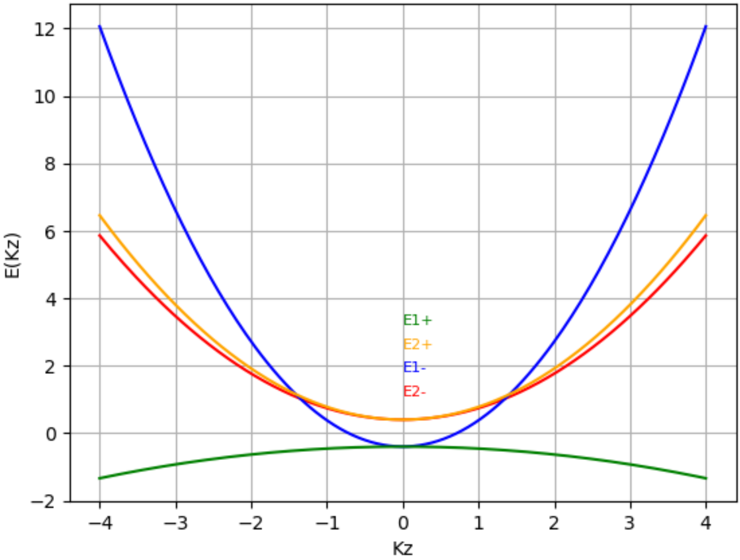


Figure: A=2.7,λ_1=1.8,λ_2=0.5,ω=20, μ=0 η=1

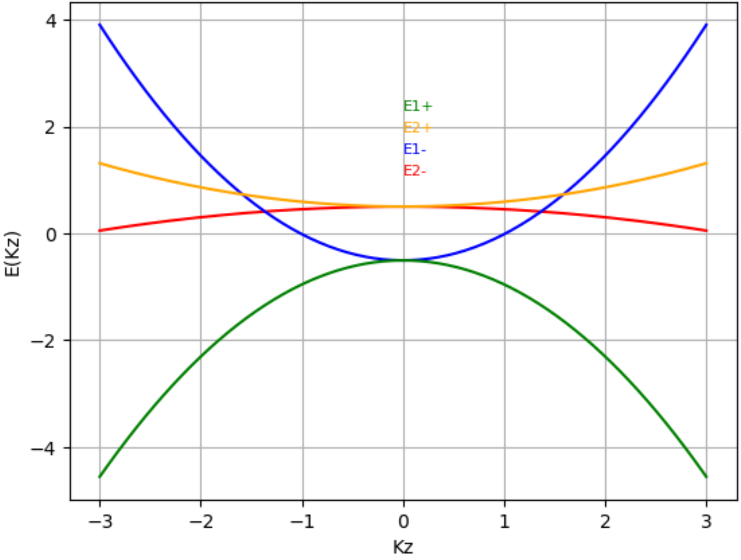


Figure: A=5,λ_1=1.8,λ_2=0.5,ω=20, μ=0 η=1

Summary

- Successful conversion of trivial semimetal to a topologically non-trivial semimetal
- Simultaneous accessibility of both types of Weyl nodes through controlled doping and tuning of laser light
- Provides another way to achieve TRS breaking Weyl semimetal using a wide variety of materials
- Adds to the repertoire of types of ways to convert a trivial semimetal to non-trivial topological semimetal(strain-induced[9], magnetic field induced[9], photo-induced[9])
- High scope of experimental realization as Luttinger Hamiltonian describes a wide variety of materials including semiconductors, pyrochlore iridates and half Heuslers which have abundant experimental samples available

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[10] Engineering topological phases in the Luttinger semimetal $\alpha - Sn$ by Dongqin Zhang et al

THANK YOU FOR YOUR ATTENTION