Understanding Dirac, Weyl and Nodal-Line Semimetals: A Step-by-Step Guide through Model Hamiltonians

Debnarayan Jana*[a], Deep Mondal[b]

Exercises

1. **Spinful, valley-resolved low–energy graphene Hamiltonian (Section III).** Work with the spinful, valley-resolved low–energy graphene Hamiltonian as shown in Section III. Briefly justify each entry (e.g. action of $T = is_yK$ and inversion exchanging A/B).

   (a) **Gap analysis at K/K'.** Show analytically that:

   - **With Rashba only** ($\lambda_R \neq 0,\ M = \lambda_{SO} = J_{ex} = 0$), the Dirac points at K/K' remain gapless. In fact, at $\mathbf{k} = 0$ one finds the spectrum

     $$\{0,\ 0,\ \pm 2\lambda_R\},$$

     so two bands remain pinned at zero energy.
   - A **Semenoff mass** M opens a trivial gap $E_g = 2|M|$ at each valley.
   - **Intrinsic SOC** λ_{SO} opens a Kane–Mele (QSHE) gap $E_g = 2|\lambda_{SO}|$ at each valley (with opposite spin masses).

   (b) **QAH from exchange + Rashba (mechanism sketch).** For $J_{ex} \neq 0$ and $\lambda_R \neq 0$ (with $M = \lambda_{SO} = 0$), explain qualitatively (or by exhibiting a lattice regularization) how a Chern gap can emerge even though each term alone is gapless: spin splitting (J_{ex}) plus spin–momentum locking (λ_R) generates a momentum–dependent mass whose sign pattern yields a nonzero Chern number once a global gap opens.

   (c) **Numerical illustration (figures with inset).** Compute and plot the pair of surfaces $\pm E(k_x, k_y)$ near a valley for three parameter sets:

   i. Gapless Rashba: ($\lambda_R > 0,\ M = \lambda_{SO} = J_{ex} = 0$);
   ii. Trivial Semenoff gap: ($M > 0,\ \lambda_R = \lambda_{SO} = J_{ex} = 0$);
   iii. Intrinsic SOC gap: ($\lambda_{SO} > 0,\ \lambda_R = M = J_{ex} = 0$).

   Scale energies to eV and add a 0–1 eV inset to each panel (zoom of the conduction branches). **Deliverable:** three figures (both conduction and valence surfaces together), consistent color scales and viewing angles, each with a 0–1 eV inset.

[0a] *Department of Physics, University of Calcutta, 92 Acharya Prafulla Chandra Road, Kolkata 700009, India. E-mail: djphy@caluniv.ac.in*
[0b] *Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India*

(d) **Edge physics expectation.**

$$\begin{aligned} M\text{-gap} &\Rightarrow \text{no net Hall effect (valley Hall only)},\\ \lambda_{SO}\text{-gap} &\Rightarrow \text{helical edges (QSHE)},\\ J_{ex}+\lambda_R &\Rightarrow \text{chiral edge(s) (QAH)}. \end{aligned}$$

Hint. At $\mathbf{k}=0$ with Rashba only, the eigenvalues are $\{0,0,\pm 2\lambda_R\}$; two bands remain at zero, hence no full gap, whereas M or λ_{SO} produce masses $\pm M$ or $\pm\lambda_{SO}$ at each valley, giving gaps $2|M|$ and $2|\lambda_{SO}|$, respectively. Readers may consult useful references [1, 2, 3, 4, 5].

2. **Continuum nodal-loop model (units $\hbar=1$).** Consider a continuum two–band Hamiltonian

$$H(\mathbf{k}) = v_x k_x \sigma_x + m(k_y,k_z)\,\sigma_z, \qquad m(k_y,k_z) = b - \sqrt{v_y^2 k_y^2 + v_z^2 k_z^2}, \tag{1}$$

with $v_{x,y,z}, b>0$ and Pauli matrices $\sigma_{x,z}$ acting in an orbital (sublattice) space. The conduction/valence energies are

$$E_\pm = \pm\sqrt{v_x^2 k_x^2 + m^2}.$$

The nodal loop lies in the (k_y,k_z) plane at $k_x=0$ and solves $m(k_y,k_z)=0$, i.e.

$$v_y^2 k_y^2 + v_z^2 k_z^2 = b^2, \tag{2}$$

an ellipse with semi–axes $a=b/v_y$ and $c=b/v_z$. Note that on the plane $k_x=0$ the Hamiltonian anticommutes with $\Gamma=\sigma_y$, i.e. $\{H(0,k_y,k_z),\Gamma\}=0$ (a chiral symmetry).

(a) **Berry (Zak) phase as a diagnostic of the drumhead region.** For each fixed (k_y,k_z), view H as a 1D insulator in k_x with “mass” $m(k_y,k_z)$. Define the Zak phase of the occupied band along k_x:

$$\phi_{\text{Zak}}(k_y,k_z) := \int_{-\infty}^{+\infty} A_x(\mathbf{k})\,dk_x, \tag{3}$$

and show

$$\phi_{\text{Zak}}(k_y,k_z) = \begin{cases} \pi, & v_y^2k_y^2 + v_z^2k_z^2 < b^2,\\ 0, & \text{otherwise.} \end{cases} \tag{4}$$

Hint. In 1D chiral Dirac, the Zak phase is π when $m<0$ and 0 when $m>0$ (mod 2π).

(b) **Berry phase on linking loops in (k_y,k_z).** Restrict to $k_x=0$ and take a small closed path C in the (k_y,k_z) plane. Show that the occupied–band Berry phase is

$$\gamma(C) = \oint_C \mathbf{A}_\parallel\cdot d\mathbf{k}_\parallel = \begin{cases} \pi, & C \text{ links the nodal ellipse once,}\\ 0, & \text{it does not link.} \end{cases} \tag{5}$$

Deliverable. Put $H(0,k_y,k_z)$ in an off–diagonal chiral form by a unitary rotation (e.g. $\sigma_z\to\sigma_x$), write

$$H = \begin{pmatrix} 0 & q\\ q^* & 0\end{pmatrix}, \qquad q \propto m(k_y,k_z),$$

and show $\gamma = \frac{1}{2}\Delta\arg q$ along C. **Hint.** A loop that winds once around a simple zero of q picks up $\Delta\arg q = 2\pi$.

(c) **Integer winding along k_x (1D invariant parameterized by (k_y, k_z)).** Show that with chiral symmetry $\Gamma\sigma_x\Gamma^{-1} = -\sigma_x$ and $\Gamma\sigma_z\Gamma^{-1} = -\sigma_z$, the 1D Hamiltonian at fixed (k_y, k_z) has a winding number

$$\nu(k_y, k_z) = \frac{1}{2\pi i}\int dk_x\, \partial_{k_x} \ln\big(d_x(k_x) - i\, m\big), \qquad d_x = v_x k_x, \tag{6}$$

and evaluate

$$\nu = \frac{1}{2}\Big(\mathrm{sgn}(m(-\infty)) - \mathrm{sgn}(m(+\infty))\Big) = \frac{1}{2}(1-1) = 0$$

unless you compactify k_x to a lattice Brillouin zone; then

$$\nu(k_y, k_z) = \begin{cases} 1, & v_y^2 k_y^2 + v_z^2 k_z^2 < b^2, \\ 0, & \text{otherwise.} \end{cases} \tag{7}$$

Hint. On a lattice, $d_x(k_x)$ winds once around the origin as k_x goes through the BZ; the sign of m decides if the loop encloses the origin.

(d) **Drumhead surface states via a mass domain wall.** Consider a slab open in x and translationally invariant in y, z. Treat k_y, k_z as parameters and replace $k_x \to -i\partial_x$. Show that when $m(k_y, k_z)$ changes sign across the surface (interior vs vacuum), there exists a normalizable zero mode localized at the surface iff $v_y^2 k_y^2 + v_z^2 k_z^2 < b^2$. Conclude that surface "drumhead" states fill the interior of the ellipse's projection. **Hint.** Solve $(-iv_x\partial_x\sigma_x + m(x)\sigma_z)\psi = 0$ with $m(x)$ kink; try $\psi(x) \propto \exp\big[-\int^x m(x')/v_x\, dx'\big]$.

(e) **Low–energy DOS (one–line scaling and prefactor).** Using tubular coordinates along the ellipse, argue that

$$\rho(E) = \frac{L_{\text{ellipse}}}{2\pi^2 v_x v_n}\, E + \mathcal{O}(E^3), \tag{8}$$

where L_{ellipse} is the ellipse circumference and v_n is the loop–average of the normal velocity $v_n = \big\|\nabla_{(k_y,k_z)} m\big\|$ on the nodal set. Check the circular limit $v_y = v_z \equiv v_\perp$ gives

$$\rho(E) = \frac{b}{\pi v_x v_\perp^2}\, E.$$

Hint. Integrate the 2D Dirac DOS density $E/(2\pi v_x v_n)$ along the nodal line. Readers may consult [6, 7, 8, 9].

References

[1] C. Kane and E. Mele, *Physical Review Letters* **95**, 226801 (2005).

[2] H. Min, J. Hill, N. A. Sinitsyn, B. Sahu, L. Kleinman, and A. H. MacDonald, *Physical Review B* **74**, 165310 (2006).

[3] A. Bandyopadyay and D. Jana, *Universal Journal of Materials Science* **8**, 32–44 (2020).

[4] L. W. Molenkamp, G. Schmidt, and G. E. W. Bauer, *Physical Review B* **64**, 121202 (2001).

[5] G. Bihlmayer, P. Noël, D. V. Vyalikh, E. V. Chulkov, and A. Manchon, *Nature Reviews Physics* **4**, 642–659 (2022).

[6] D. Vanderbilt, *Berry Phases in Electronic Structure Theory: Electric Polarization, Orbital Magnetization and Topological Insulators*, Cambridge University Press (2018).

[7] D. Mondal, A. Bandyopadhyay, A. Nandy, and D. Jana, *Applied Materials Today* **40**, 102360 (2024).

[8] D. Mondal, A. Bandyopadhyay, and D. Jana, *International Journal of Theoretical Physics* **64**, 1–34 (2025).

[9] Y. H. Chan, C.-K. Chiu, M.-J. Chou, and A. P. Schnyder, *Physical Review B* **93**, 205132 (2016).