Thermo-electric transport in Landau Quantized Hall States of a multi-Weyl Semimetal

Anirudha Menon\textsuperscript{1} and Banasri Basu\textsuperscript{2}

\textsuperscript{1}Department of Physics, University of California, Davis, California 95616, USA\textsuperscript{*}
\textsuperscript{2}Physics and Applied Mathematics Unit, Indian Statistical Institute, Kolkata 700108, India\textsuperscript{†}

(Dated: January 23, 2019)

We study the effect of a perpendicular magnetic field $\mathbf{B}$ on a multinode Weyl semimetal (mWSM) of arbitrary integer monopole charge $n$, with the two Weyl multinodes separated in k-space. Besides type-I mWSMs, there exist type-II mWSMs which are characterized by the tilted minimal dispersion for low-energy excitations; the Weyl points in type-II mWSMs are still protected crossings but appears at the contact of the electron and hole pockets, after the Lifshitz transition. We find that the presence of a perpendicular magnetic field destroys this feature due to the Landau quantization. In this theory, the Hilbert space is spanned by a set of $n$ chiral degenerate ground states, and a countably infinite number of achiral Landau levels. We calculate the Hall conductivity for the tilt-symmetric case in the zero frequency limit, and show that the exact $T \to 0$ expression generalizes from the formula for elementary ($n=1$) type-I WSMs, using the permutation operator. Only one of the $n$ zero modes contribute to Hall transport, such that the node separation contribution is annihilated. We derive a universal expression (valid for arbitrary $n$) for the type-II mWSM Hall conductivity which is bounded by a Landau level cutoff, introduced on physical grounds and analogous to the momentum cutoff for the $B=0$ case. The corresponding thermal Hall and Nernst conductivities are evaluated and characterized. This work is intended to classify the properties of generic mWSMs into two equivalence classes, modulo the topological Lifshitz transition.

\textbf{Introduction.} In Quantum field theories, fermions are described by four-component spinors which obey the Lorentz invariant Dirac equation. In the massless limit, a single Dirac spinor decouples to two two-component Weyl spinors \cite{1,2} called Weyl or chiral fermions. In recent years, the otherwise elusive Weyl fermions have been realized in condensed matter physics through table top experiments \cite{3–5}, and find theoretical generalizations to a class of quasi-particles characterized by topological invariants, called multi-Weyl semimetals \cite{6–8}.

A generic multi-Weyl semimetal (mWSM) is considered to be a topological quantum system, with two k-space monopoles having opposite topological charge, and a gapless spectrum \cite{9,10}. The integer charged monopoles occur in pairs and act as a source or sink for the Berry flux, i.e., the surface integral of the $\mathbf{U}(1)$ Berry 2-form \cite{11,12}. These monopoles constitute the Weyl nodes, which are the points at which the valence and conduction bands touch. The low energy description involves minimal models for a mWSM, which require either inversion or time-reversal symmetry to be broken \cite{13–15}, and give rise to Dirac-like dispersions at the Weyl nodes along a symmetry direction. The remaining directions contribute to the energy non-linearly, dictated by the monopole charge, leading to anistropy \cite{6,8,12}.

Weyl nodes of opposite chirality merge and annihilate in pairs, while those of the same chirality can merge to form nodes of larger topological charge, which are stable provided that there is a point group symmetry protecting the merger \cite{6,9,10}. One can then understand the mWSM as a robust state of mergers of $n$ like-chirality unit charge monopoles or elementary WSMs. Elementary WSMs have been examined both theoretically and experimentally in the context of chiral magnetic waves \cite{16}, chiral anomaly induced plasmon modes \cite{17}, magneto-optical transport \cite{18}, and negative magneto-resistance \cite{19}.

In the low energy description, a Lorentz symmetry violating tilt (C) term can be used to induce a new phase of elementary WSMs known as type-II mWSMs \cite{20}, with $C \gg v$, $v$ being the Fermi velocity. Materials with this band-structure have quasi-particle pocket Fermi surfaces at charge neutrality, compared to the point like Fermi surfaces for type-I WSMs ($C \ll v$). This construction can be extended \cite{21} to WSMs of arbitrary winding number and can be used to probe the properties of type-II mWSMs sufficiently far away from the topological Lifshitz transition separating the two phases.

Recent experimental reports claim the discovery of SiS\textsubscript{2} \cite{7} and HgCr\textsubscript{2}Se\textsubscript{4} \cite{9,10} as possible candidates for mWSMs with monopole charge $n=2$. The dispersion anisotropy in mWSMs coupled with spin-momentum locking \cite{6} has the potential to give rise to unique transport signatures in the form of the chiral anomaly \cite{16,17}, for $n=1$), anisotropic screening of Coulomb interactions \cite{22}, for $n=1$), and topological Hall physics \cite{13}, for $n=1$). These materials are thought to differ in these properties from the elementary WSMs, i.e., with $SO(2)$ symmetric dispersion relations.
Motivated by the prospect of rich and novel physics, we study the static Hall conductivity of a mWSM in a perpendicular magnetic field (explored in the $n = 1$ type-I WSM case [23]), for both type-I and type-II WSMs in this letter. We find that under the influence of a perpendicular magnetic field, the continuum band-structure of the minimal model mWSM splits into discrete copies of one-dimensional dispersions in a plane perpendicular to the direction of quantizing field. The degenerate ground states of this system are chiral, as a recent experimental study [24] indicates, leading to interesting consequences on Hall transport. Additionally, Mott’s relations [13, 18] permit the study of the thermal Hall and Nernst conductivities, and we discuss the implications of arbitrary Chern number on all these material properties.

The paper is structured as follows: We begin by diagonalizing the minimal time-reversal symmetry breaking model of an mWSM in a perpendicular magnetic field and discuss the underlying physics of corresponding Landau levels. We explore the implication of the chiral zero modes induced by the topological transition of the mWSM electronic structure, due to the presence of the quantizing field, on the off-diagonal transport properties of the system. Additionally, results for type-I and type-II thermal Hall and Nernst conductivities are stated and explained in the context of the underlying dispersion and occupations. We make a few remarks about possible experimental validation of our work, and sum up our findings.

The Model. Our discussion begins with the minimal Hamiltonian for a pair of multi-Weyl (mW) nodes given by

$$H_s^t = \hbar C_s (k_z - sQ) + sh_v a_n \mathbf{\sigma} \cdot \mathbf{n}_p,$$  \hspace{1cm} (1)

where $s = \pm$ characterizes the WP, $C_s$ is the tilt parameter, which can be different for each node, in principle. Here, $\mathbf{n}_p = \frac{1}{2} \left[ p_{y}^n \cos(n \phi_p), p_{x}^n \sin(n \phi_p), \frac{v(p_z - s h)}{\alpha_n} \right]$, $p_{\perp} = \sqrt{p_{y}^2 + p_{x}^2}$, $\mathbf{\sigma}$ is the vectorized Pauli matrix, $v$ denotes the Fermi velocity in the absence of tilt, and $n$ is the monopole charge. This Hamiltonian has mW nodes separated by $2Q$ along $e_z$, which is the unit vector along the $z$-direction in momentum space, and $\alpha_n$ constitutes the dimensionally consistent generalization of the Fermi velocity in the $k_x - k_y$ plane.

We proceed by introducing a magnetic field perpendicular to the $x - y$ plane in the Landau gauge: $\mathbf{A} = B \times \mathbf{y}$ such that $\mathbf{B} = \nabla \times \mathbf{A} = -B \mathbf{z}$. The Hamiltonian is presented in the compact matrix form:

$$H_{s,B}^n = \begin{bmatrix} (C_s + sv)z & i^n s \frac{2a}{B} (\sqrt{2}a)^n \\ -i^n s \frac{2a}{B} (\sqrt{2}a)^n & (C_s - sv)z \end{bmatrix},$$  \hspace{1cm} (2)

with the introduction of the ladder operators $a(a^\dagger)$, following the Pierel’s substitution $p_i \rightarrow p_i - c A_i$, and setting $c = 1$, $h = 1$, $z = k_z - sQ$. The spectrum $E_{N}^{s,t}$ and eigenstates of the mW Hamiltonian for the Landau levels $N \geq n$ are given by [25]

$$E_{N}^{s,t} = C_s z + tv \sqrt{z^2 + N P_n \Omega^2}$$  \hspace{1cm} (3)

$$| N, s, t, k_z \rangle = \begin{bmatrix} C_{t,s,t,k_z,N} \langle N \rangle \\ C_{s,t,k_z,N} \langle N - n \rangle \end{bmatrix},$$  \hspace{1cm} (4)

![FIG. 1: (a) Left panel: Spectrum of a type-I mWSM in the absence of a magnetic field. Right panel: Tilted type-II mWSM spectrum with $B = 0$, showing the formation of electron and hole pockets characteristic of this phase. (b) Left panel: Type-I mWSM spectrum in the presence of a perpendicular magnetic field. The achiral valence and conduction bands are in green and red respectively, with the Fermi surface shown in yellow, while the chiral bands are depicted in blue. Right panel: Type-II mWSM with tilted bands showing that every LL $N$ is partially occupied.](image)

where, $\Omega$ represents the LL spacing [25]. The eigenstates have been unit-normalized, and the quantum number $t = \pm(-)$ denotes the conduction (valence) bands, equivalently called the valley degrees of freedom.
Here, the dependence of the wavefunctions on the plane waves in the $y$ and $z$ directions have been suppressed for brevity, and since the dispersion has no explicit dependence on $k_y$, it is macroscopically degenerate. The Landau levels, characterized by $N$ in the elementary WSM case, now generalize to $NP_n$, where $P$ is the permutation operator.

The modes with $0 \leq N \leq n - 1$ take the form

$$|N = n - q, s, k_z, s \cdot t = +\rangle = \left[ \begin{array}{c} n - q \\ 0 \end{array} \right],$$

$$1 \leq q \leq n, \quad q \in \mathbb{N}, \quad (5)$$

and are chiral since the $s \cdot t = -1$ states vanish [25]. These states are also degenerate and their number equals the monopole charge $n$.

**Band-Structure of Minimal Model.** In the absence of a magnetic field, the dispersion of the $s = + (Q = 0, C_+ = C > 0)$ node of a mWSM is given by [8, 12]

$$E_y(k) = Ck_z + tv\sqrt{k_x^2 + \gamma^2(k_x^2 + k_y^2)^n}, \quad (6)$$

where $t$ represents the valley degree of freedom, $\gamma$ is a dimensionful constant (given by $\gamma = \alpha_n/v$), and $v$ is the Fermi velocity. The bands for type-I mWSMs ($C \ll v$) are shown as a function of $k_z$ in Fig. 1(a) (left) and form a continuum with the actual band-structure presenting finite electron pockets at $\mu > 0$, while the minimal model dispersion gives rise to infinite electron pockets near the Lifshitz transition. For type-II WSMs, the tilt ($C \gg v$) leads to the creation of electron and hole pockets which are also unbounded [shown in Fig. 1(a) (right)] in the minimal model, leading to the requirement of a physical cutoff of the LL contribution.

The presence of a magnetic field causes the band-structure to change dramatically [25] with one-dimensional profiles in the $E - k_y$ planes for each Landau level $N$, as shown in Fig. 1(b) (left) with the valence and conduction bands being increasingly gapped for $N \geq n$. The blue line depicts the $n$ degenerate zero-modes which are chiral, and all the LLs have point-like Fermi surfaces which are characteristic for type-I WSMs. As the Lifshitz phase transition is approached by tilting the spectrum, the number of LLs which are occupied grows in an unbounded manner [13, 18], and the minimal model becomes singular at the Lifshitz point, $C = v$.

As we move away from the Lifshitz transition into the type-II mWSM regime, the Fermi surface remain point-like for all states [Fig. 1(b) (right)]. This remarkable feature can be understood in terms of the 1d profiles for each LL (band) induced by the perpendicular magnetic field, instead of the electron and hole pockets [Fig. 1(b)] found in the 3d continuum dispersion for the $B = 0$ states of a mWSM. The unbounded electron and hole pockets can lead to divergent momentum integrals in the evaluation of transport coefficients, and are usually treated in the minimal model mWSM by introducing a momentum cutoff, $\Lambda$. By analogy, in the case of the Landau quantized mWSM, it turns out that the minimal model based calculations receive contributions from every one of the infinite LLs in the type-II mWSM phase. Physically, of course, these contributions must be finite, and so we propose that the contribution from the LLs be cutoff at some $N_{max} \gg 25$, which is the analogue of $\Lambda$. The electron and hole pockets reappear in the $B \to 0$ limit as the integer valued $N$-axis, scaled by $B$, gets squeezed into a continuum.

We pursue the calculation of zero frequency DC Hall conductivity tensor in the linear response regime and use the Kubo formula in $d = 3$ for brevity, and since the dispersion has no explicit dependence on $k_y$, it is macroscopically degenerate. The Landau levels, characterized by $N$ in the elementary WSM case, now generalize to $NP_n$, where $P$ is the permutation operator.

$$\sigma_{\alpha\beta}(\omega) = -\frac{i}{2\pi f_B^2} \sum_{N,N',t,t'} \int \frac{dk_z}{2\pi} f^+_{N,k_z,t} - f^+_{N',k_z,t'} \langle N,t,s | J_\alpha | N',t',s \rangle \langle N',t',s | J_\beta | N,t,s \rangle \omega - E^+_N + E^+_N - i\eta$$

where $J_\alpha(\beta)$ represents the current operator, $|N,t,s\rangle$ are the states, and $f^+_{N,k_z,t}$ is the Fermi-Dirac distribution. In general, the Mott’s relationship [13, 18] defines the thermal Hall and Nernst conductivities as

$$\alpha_{xy} = eLT \frac{\partial \sigma_{xy}}{\partial \mu}, \quad K_{xy} = LT \sigma_{xy}, \quad (8)$$

where $L = \pi^2 k_B^2/3e^2$ is the Lorentz number, $e$ is the electronic charge, and $k_B$ is the Boltzmann constant. The Hall conductivity tensor can be computed analytically in the $T \to 0$ and $\omega \to 0$ (DC) limit, for both type-I and type-II mWSMs, in the tilt-symmetric case $C_+ = -C_- = C > 0$ [25].

**Type-I mWSM Hall conductivity.** In this case, the computation of the off-diagonal component of the conductivity tensor yields,
\[ \sigma_{xy} = \frac{e^2}{4\pi^2} \frac{v}{v^2 - C^2} \left[ n\mu + \sum_{N=n}^{N_{\text{max}}} [\mu^2 - \Omega^2 (v^2 - C^2)^N P_n]^{1/2} \right]. \tag{9} \]

Of the degenerate \( n \) ground states, only the \(|n - 1| \) chiral mode contributes to the Hall conductivity with the remaining modes being inert. Since the contributing ground state is chiral, the node separation term, present in the \( B = 0 \) case, is annihilated \([25]\). Under the circumstance that only the ground state is occupied, the Hall conductivity scales as the monopole charge, which can be interpreted as the contribution of \( n \) Fermi arcs connecting \( n \) pairs of (unit monopole charge) Weyl point \([6]\). This description breaks down for the higher LLs where the functional dependence is more complicated. Increasing \( \mu \) from charge neutrality gives discontinuous jumps in Hall conductivity as higher LLs get occupied which is a hallmark of quantum Hall phases.

The expression for \( \sigma_{xy} \) becomes singular as \( C \to v \), a consequence of the appearance of infinite LL contributions in the minimal model when approaching the Lifshitz transition form the mWSM-I side. As in the zero-field elementary WSM case, the expression for the \( \sigma_{xy} \) is independent of the cutoff. The thermal Hall and Nernst conductivities are plotted as a function of magnetic field \([\text{Fig. 2 (a)}]\) and chemical potential \([\text{Fig. 2 (b)}]\).

**Type-II mWSM Hall conductivity.** The results for type-II mWSMs are as follows \([25]\):

\[ \sigma_{xy} = \frac{e^2}{4\pi^2} \frac{C}{C^2 - v^2} \left[ n\mu \frac{C}{v} + 2\mu (N_{\text{max}} + 1 - n) \Theta(N_{\text{max}} + 1 - n) \right], \tag{10} \]

with \( N_{\text{max}} \) \([25]\) being the physically motivated cutoff of the LL occupation. To the best of our knowledge, this is a new result which has not been computed prior to this work, even for \( n = 1 \). Noticeably, the Hall conductivity vanishes for \( \mu = 0 \), with the first term being identical to eqn. \((9)\) to leading order in \( v/C \). The Hall conductivity grows linearly with increasing \( v/C \). The evaluation of the cutoff. While increasing \( \mu \) in the minimal model has no effect on occupation since all the LLs are occupied, real materials will experience an increasing quasi-particle occupations corresponding to an increasing physical cutoff, \( N_{\text{max}} \). The variation of thermal Hall and Nernst conductivities with tilt and Fermi velocity are depicted in Fig. 3 (a) & 3(b).
and can be measured directly. The system’s response to a current in the linear regime, and thermal Hall coefficients calculated here represent topologically non-trivial systems [29–31]. The Nernst conductivity of transport properties of materials in general, not just classes of setups are fairly common for the measurement claims made in this letter, i.e, eqns. (9) & (10). Such closed circuit setup [13, 18] can be used to verify the zero mode thermal Hall conductivity which has peaks corresponding to the occupation of new LLs.

The chirality of the zero mode that contributes to the Hall conductivity leads to the destruction of the node separation \((Q)\) contribution to the Hall conductivity in both type-I and type-II mWSMs, unlike the \(B = 0\) cases. The type-I Hall conductivity generalized from the \(n = 1\) case [22], and varying the chemical potential causes jumps in the Hall conductivity, as more states are occupied. This feature is also reflected in the Nernst conductivities which has peaks corresponding to the occupation of new LLs.

For type-II WSMs, both the zero mode thermal Hall and Nernst conductivities are boosted by a factor of \(\frac{C}{v}\), and get contributions from all of the countably infinite LLs, which is a feature of the minimal model in the \(B \neq 0\) case. This motivates the introduction of a LL cutoff, similar in spirit to the standard momentum cutoff introduced in the \(B = 0\) case, since the responses of physical materials are finite. The Nernst conductivity remains a constant up to a change in the cutoff \(N_{\text{max}}\) dictated by the Fermi level. The qualitative and quantitative observations made in this letter are designed to serve in the characterization of generic mWSMs of both types, putting their properties in an equivalence class modulo the two types of tilt.

**Conclusion.** In this letter, we have considered the effects of a perpendicular magnetic field on generic type-I and type-II multi-Weyl Semimetals. We have analyzed the structure of the Hilbert space, and computed the Hall conductivity tensor in the linear response regime using the Kubo formula in the zero frequency limit.

We find that the Hilbert space, in the presence of the quantizing field, hosts \(n\) zero modes which are both degenerate and chiral, while the higher Landau levels are achiral. Interestingly, the appearance of the electron and Hall pockets, which is a hallmark of type-II WSM physics, get destroyed in the presence of this perpendicular field. The continuum pocket construction manifests itself through infinite LL occupation in this case. Of the \(n\) chiral zero modes, only the \(|n - 1|\) state contributes to the Hall conductivity while the remaining \(n - 1\) ground states remain inert.

The anisotropic dispersion of a general mWSM close to the Weyl node in the presence of a perpendicular magnetic filed can be confirmed using angle-resolved photo-emission spectroscopy [27, 28]. Also, a simple closed circuit setup [13, 18] can be used to verify the claims made in this letter, i.e, eqns. (9) & (10). Such classes of setups are fairly common for the measurement of transport properties of materials in general, not just topologically non-trivial systems [29–31]. The Nernst and thermal Hall coefficients calculated here represent the system’s response to a current in the linear regime, and can be measured directly.

---

[1] M. E. Peskin and D. V. Schroeder, An Introduction to quantum field theory, Reading, USA: Addison-Wesley (1995).
[2] H. Weyl, I.Z. Phys 56(5), 330-352 (1929)
[3] B. Q. Lv, H. M. Weng, B. B. Fu, X. P. Wang, H. Miao, J. Ma, P. Richard, X. C. Huang, L. X. Zhao, G. F. Chen, Z. Fang, X. Dai, T. Qian, and H. Ding, Phys. Rev. X 5, 031013 (2015).
[4] Shuang Jia, Su-Yang Xu, M. Zahid Hasan, ArXiv: 1612.00416v2 (2016).
[5] Su-Yang Xu et al., Science 349 6248 (2015).
[6] S. Ahn, E. J. Mele, and H. Min, Phys. Rev. B 95, 161112(R) (2017).
[7] Shin-Ming Huang et al., PNAS 113, 5 (2016)
[8] Yong Sun and An-Min Wang, Phys. Rev. B. 96, 085147 (2017).
[9] G. Xu, H. Wend, Z. Wang, X. Dai, and Z. Fang, Phys. Rev. Lett. 107, 186806 (2011).
[10] C. Fang, M. J. Gilbert, X. Dai, and B. A. Bernevig ], Phys. Rev. Lett. 108, 266802 (2012).
[11] "The Quantum Hall Effect", D. Tong, ArXiv: 1606.06687v2.
[12] R. M. A. Dantas, F. Pena-Benitez, B. Roy, and P. Surowka, JHEP 12, 069 (2018).
[13] Y. Ferreiros, A. A. Zyuzin, and Jens H. Bardarson, Phys. Rev. B 96, 115202 (2017).
[14] A. A. Burkov and L. Balents, Phys. Rev. Lett 107, 127205 (2011).
[15] G. B. Halasz and L. Balents, Phys. Rev. B 85, 035103 (2011).
[16] D.E. Kharzeev and H.-U. Yee, Phys. Rev. D 83, 085007 (2011).
[17] J. Zhou, H.-R. Chang, and D. Xiao, Phys Rev. B. 91, 035114 (2015).
[18] A. Menon, D. Chowdhury, B. Basu, Phys. Rev. B 98, 205109 (2018).
[19] H. Nielsen and M. Ninomiya, Phys. Lett. B 130, 389 (1983).
[20] A. A. Soluyanov, D. Gresch, Z. Wang, Q. Wu, M. Troyer, X. Dai, and B. A. Bernevig, Nature 527, 495-498 (2015).
[21] M. Breitkreiz, N. Bovenzi, and J. Tworzydo, Phys. Rev. B 98, 121403(R) (2018).
[22] J. Klier, I. V. Gornyi, and A. D. Mirlin, Phys. Rev. B 96, 214209 (2017).
[23] P. Hosur, S. A. Parameswaran, and A. Vishwanath, Phys. Rev. Lett. 108, 046602 (2012).
[24] X. Yuan et.al., Nat. Comm. 9, 1854 (2018).
[25] See Supplementary Material. In Appendix A, we present the spectrum of the system. Appendix B contains the generalities regarding the Kubo formula. We sketch the Hall conductivity calculation for type-I and type-II mWSMs in Appendix C and Appendix D respectively. In Appendix E, we show the numerical verification of the geometric structure of the dispersion. Appendix F provides a numerical proof of the uniqueness of the $N_{max}$.
[26] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982).
[27] M. Sentef, A. F. Kemper, B. Moritz, J. K. Freericks, Z.-X. Shen, and T. P. Devereaux, Phys. Rev. X 3, 041033 (2013).
[28] H. Hubener, M. A. Stenef, U. De. Giovannini, A. F. Kemper, and A. Rubio, Nat. Commun. 8, 13940 (2017).
[29] M. Hirschberger, S. Kushwaha, Z. Wang, Q. Gibson, S. Liang, C. A. Belvin, B. A. Bernevig, R. J. Cava, and N. P. Ong, Nat. Mater. 15, 1161 (2016).
[30] F. C. Chen, H. Y. Lv, X. Luo, W. J. Luo, W. J. Lu, Q. L. Pei, G. T. Lin, Y. Y. Han, X. B. Zhu, W. H. Song, and Y. P. Sun, Phys. Rev. B 94, 235154 (2016).
[31] J. Gooth, A. C. Niemann, T. Meng, A. G. Grushin, K. Landsteiner, B. Gotsmann, F. Menges, M. Schmidt, C. Sekhar, V. SuB, R. Huhne, B. Rellinghaus, C. Felser, B. Yan, and K. Nielsch, Nature (London) 547, 324 (2017).