Dirac dispersion generates unusually large Nernst effect in Weyl semimetals
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ABSTRACT

Weyl semimetals contain linearly dispersing electronic states, offering interesting features in transport yet to be thoroughly explored thermally. Here we show how the Nernst effect, combining entropy with charge transport, gives a unique signature for the presence of Dirac bands and offers a diagnostic to determine if trivial pockets play a role in this transport. The Nernst thermopower of NbP exceeds its conventional thermopower by a hundredfold, and the temperature dependence of the Nernst effect has a pronounced maximum. The charge neutrality condition dictates that the Fermi level shifts with increasing temperature toward the energy that has the minimum density of states (DOS). In NbP, the agreement of the Nernst and Seebeck data with a model that assumes this minimum DOS resides at the Dirac points is taken as strong experimental evidence that the trivial (non-Dirac) bands play no role in high-temperature transport.
Unique features intrinsic to Weyl semimetals (WSM) lead to interesting galvanomagnetic transport phenomena [1,2]. Preliminary theoretical studies predict that bulk Weyl nodes [3,4] and surface Fermi arcs [5] have magnetothermal and thermomagnetic transport signatures beyond classical semimetal electrical transport signatures. Dirac fermion experimental thermomagnetic data exists [6,7], including magnetic-field-dependent adiabatic Seebeck coefficients [8,9]. While model fits to data exist for PbSnSe [6] and Cd₃As₂[7], here we present a quantitative understanding of the NbP Nernst and Seebeck coefficients without recourse to fitting parameters for temperature or field dependences.

We show that symmetry between the electron-like and hole-like Dirac band portions results in (i) a characteristic temperature- and magnetic-field-dependent Nernst thermopower, and (ii) a relation between the Nernst and Seebeck coefficients’ unique Dirac band signatures. We report and explain the single-crystal NbP isothermal Nernst and magneto-Seebeck effects on samples with large, unsaturated magnetoresistances and ultrahigh mobilities. In the zero-temperature limit the NbP band structure has 24 Weyl points and several trivial pockets [2]. Here we show that with increasing temperatures, electrons/holes in the NbP symmetric Dirac bands dominate transport as electrochemical potential \( \mu(T) \) moves toward the Dirac point, minimizing contributions from the trivial bands (i.e., no Dirac dispersion near the electrochemical potential).

The Nernst effect is a decreasing function of temperature in classical, non-Dirac semimetals like Bi [10], except in the phonon-drag regime, excluded here [9]. In NbP, the Nernst effect temperature dependence is non-monotonic with a maximum at \( T_M \). The experimental Nernst thermopower is two orders of magnitude larger than the Seebeck coefficient. We show these two effects as specific to Dirac bands. When electrons and holes coexist in equal density in symmetric bands, the Seebeck coefficient tends to zero and the Nernst effect (the sum of the electron and hole contributions [11]) is large. Furthermore, the local charge-neutrality condition in undoped semiconductors and semimetals dictates that \( \mu(T) \) is located at the energy where the density of states (DOS) is minimal. When defects or aliovalent impurities add an extrinsic charge-carrier density, \( \mu(T) \), in the limit \( T \to 0K \), falls in a band at \( \mu_0 \). As the temperature increases such that thermally-induced intrinsic charge carriers outnumber extrinsic carriers, \( \mu(T) \) tends toward the energy minimizing DOS. We demonstrate that in NbP, this energy is the Dirac point of the carriers in the W2 band identified in Ref [2], which we define as the energy scale zero. This claim is based on a model using independently derived values for the parameter \( \mu_0 \) and the carrier scattering time \( \tau \), applying no fitting parameters. In this model, the Nernst coefficient first
increases with increasing temperature for \( T<T_M \) as \( \mu(T) \) starts from \( \mu_0 \) and tends toward the Dirac point, thereby increasing compensation between electrons and holes. For \( T>T_M \), the Nernst coefficient decreases as the Fermi distribution broadens with increasing temperature and the relative contribution of non-linear band dispersions increases. Simultaneously, the Seebeck coefficient for \( T>T_M \) tends to zero due to compensation in the dispersion. This model tracks experiments quantitatively and qualitatively, providing strong evidence that Dirac bands dominate conduction and \( \mu(T) \) reaches the Dirac point at \( T=T_M \). We conclude that the trivial bands contribute little to transport at high temperature \( (T>T_M) \) in NbP. Similar temperature dependences are observed in experimental Nernst coefficients of other Weyl semimetals, indicating similar behavior, although this must be investigated individually.

The maximum Nernst thermopower found, \( \alpha_{xyz}(9T, 109K) \sim 800 \mu\text{V/K} \), is remarkable, surpassing traditional thermoelectric semiconductors’ thermopower \( \sim 200–300 \mu\text{V/K} \). Developing materials where this happens near room temperature would be technologically significant because output from a transverse Nernst thermoelectric generator or Ettingshausen cooler scales intrinsically with device size [12,13], does not require separate n- and p-type legs, and functions over large temperature differences without staging or cascading, offering advantages over conventional thermoelectric modules.

With magnetic-field application along the \( z \)-axis \(<001> \) and temperature gradient perpendicular along the \( x \)-axis, the isothermal Nernst thermopower \( \alpha_{xyz} \) is the transverse electric field measured along the \( y \)-axis. The isothermal Seebeck coefficient \( \alpha_{xxz} \) measures longitudinal electric field along the \( x \)-axis:

\[
\alpha_{xyz} \equiv \frac{E_y(H_z)}{-\nabla_x T} \bigg|_{V_y,T=0} ; \quad \alpha_{xxz} \equiv \frac{E_x(H_z)}{-\nabla_x T} \bigg|_{V_y,T=0} \tag{1}
\]

The Nernst coefficient is defined as \( N_{xyz} \equiv \frac{d\alpha_{xyz}}{dH} \bigg|_{V_y,T=0,H_z} \). Unlike prior work [9], we study these quantities \textit{isothermally}, such that \( \nabla_y T = 0 \) [14]. The distinction between isothermal and adiabatic thermomagnetic transport is fundamental [14] and detailed in the supplement [15]; transport theory models isothermal coefficients, not adiabatic ones.

Previous two-band Drude models fit electrical transport in compensated semimetals well, e.g., \( \text{Pb}_{1-x}\text{Sn}_x\text{Se} \) [6] and \( \text{WTe}_2 \) [16]. Nevertheless, we present a WSM Hamiltonian-based theory [17], which does not invoke each band contribution in a multiband system, but instead, an integral covering energies lower and higher than that of the Dirac point. Fig. 1(a) plots the energy band structure. Fig. 1(b) gives a two-dimensional picture of one Dirac band. The model is solved self-
consistently for $\mu(T)$, which moves to the nodal energy with increasing temperature on a scale of $T/\mu_0/k_B$, Fig. 1(c). This hypothesized $\mu(T)$ behavior ignores any trivial band contribution and is crucial to the temperature-dependent Nernst effect. The supplement [15] provides thermomagnetic tensor-element calculations from the WSM Hamiltonian in the Boltzmann formalism, and calculates the isothermal Seebeck and Nernst coefficients as a function of magnetic field and temperature. The linear Dirac band dispersion results in a quadratic dependence of the DOS’s energy dependence. If the relaxation time also has an energy dependence that is a power law of energy, $\tau(\varepsilon) = \tau_0 \varepsilon^{\lambda}$ with $\lambda$ an integer, the Fermi functions entering the integrals at zero magnetic field have analytical solutions, obviating the need for the Bethe-Sommerfeld expansion [18], valid only in the degenerate limit. Therefore, analytic solutions can be derived for the thermopower and the low-field Nernst coefficient of symmetric Dirac bands, valid at all temperatures. For $\lambda=0$ (energy-independent relaxation time), they are:

$$\alpha_{xx} = \frac{2\pi^2}{3} \frac{k_B}{e} \frac{\mu}{k_B T} \left[ \frac{k_B T}{\mu} \right]^2 \frac{1 + \left( \frac{k_B T}{\mu} \right)^2}{1 + \frac{\pi^2}{3} \left( \frac{k_B T}{\mu} \right)^2} \left( \frac{k_B T}{\mu} \right)^2$$

$$\lim_{H_x \to 0} N_{xyz} = \frac{\pi^2}{3} \frac{\nu_F}{T} \left[ \frac{k_B T}{\mu} \right]^2 \frac{1 + \left( \frac{k_B T}{\mu} \right)^2}{1 + \frac{\pi^2}{3} \left( \frac{k_B T}{\mu} \right)^2} \left( \frac{k_B T}{\mu} \right)^2$$

(2).

These functions quantitatively describe most of the important features of the low-field Nernst and Seebeck coefficients including the non-monotonicity of the temperature dependence. They predict that the low-field Nernst coefficient will maximize at $T_{ML} \approx \sqrt{\frac{3}{\pi}} \frac{\mu_0}{k_B}$, above which it will decrease following a $1/T$ law. The Nernst coefficient high-field slope must be derived from numerical calculations in the supplement [15] and will have a maximum at $T_{ML} \approx \frac{\mu_0}{k_B}$. Theory still requires that two parameters, $\mu_0$ and $\tau$, be quantitative. Comparing theory and experiment, these will be derived independently from the experimental Nernst and Seebeck coefficients: $\mu_0$ from de Haas-van Alphen (DHVA) and Shubnikov-de Haas (SDH) oscillations, and $\tau$ from resistivity.

This work experimentally characterizes a 2.25 x 1.29 x 0.52 mm single crystal of NbP, made following Ref. [2] and fully characterized with resistivity, thermal conductivity, specific
heat, and magnetization (see supplement [15]), confirming the crystal had properties similar to that in Ref [2]. The sample was mounted on a silicon backing plate with a temperature gradient applied along \( x \) and magnetic field along \( z <001> \). Measurements follow the conventions of Eq. 1 with \((x,y,z)\) coordinates orthonormal \((x\ and \ y \ orientations \ lie \ unidentified \ in \ the \ <001> \ plane)\).
The silicon plate underlying the sample thermally short-circuits it so that the temperature gradient established in the silicon also is imposed on the NbP with \( \nabla_y T \approx 0 \), which is an isothermal mount. This is mounted in the Thermal Transport Option on a Quantum Design Physical Property Measurement System modified for isothermal Nernst and Seebeck measurements. This mount differs from the manufacturer-recommended conventional adiabatic mount used in Ref. [9]. The supplement [15] shows theoretically and experimentally the difference between isothermal and adiabatic measurements. For emphasis, this difference cannot be eliminated by data post-processing, such as by symmetrizing even and odd in-field parts.

The experimental Nernst effect results are shown in Figs. 2(a) (magnetic field dependence of Nernst thermopower) and 3(a) (temperature dependence of Nernst coefficient). \( \alpha_{xyz} \) is an odd function of \( H_z \) with a higher slope near zero magnetic field than at high field. We see a large, unsaturated Nernst thermopower with a maximum exceeding 800 \( \mu \)V/K at 9T, 109K. The Nernst coefficient temperature dependence taken at low field (\(|H_z|<2T|\)) and at high field (3T<\(|H_z|<9T|\)) are non-monotonic, with a maximum around \( T_{ML} \approx 55\pm 10K \) for low-field and \( T_{MH} \approx 90\pm 10K \) for high-field, consistent with the model prediction \( T_{ML} \approx \sqrt{3/\pi} T_{MH} \). The Fig. 3(a) inset shows the Seebeck coefficient \( \alpha_{xxz} \) temperature dependence; \( \alpha_{xxz} \) is nearly two orders of magnitude smaller than the maximum 9T Nernst thermopower, and its absolute value is much smaller than the high-field Nernst effect at all temperatures. The \( \alpha_{xxz} \) temperature dependence has a broad minimum around \( T_{MS} \approx 60-100K \). No \( \alpha_{xxz}(H_z) \) magnetic-field dependence is observed within instrument sensitivity. This result does not contradict prior measurements [9] of the adiabatic magneto-Seebeck coefficient; those reflect an \( \alpha_{xyz} \) contribution due to a finite \( \nabla_y T \) induced by a thermal Hall effect resulting from the adiabatic measurement technique (see supplement [15]).

To compare theory to experiment quantitatively, we determine first the Fermi level value, \( \mu_0 \), setting the temperature scale. At low temperatures (Fig. 2(a) inset), the Nernst thermopower exhibits SDH oscillations. The periods observed in SDH and DHVA oscillations in the magnetization (see supplement [15]) correspond well within our measurement error bars to those of Ref. [19]. These periods are used in conjunction with density functional theory (DFT) to derive \( \mu_0 \)'s position vis-à-vis the Weyl points in the 0K limit. DFT calculations were performed using the
Vienna *ab-initio* Simulation Package [20] with a generalized gradient approximation [21]. The tight-binding model Hamiltonian was calculated by projecting Bloch states onto maximally localized Wannier functions [22] used for generating Fermi surfaces. In the 0K limit, there are two Weyl-point types in NbP: one in the $k_z=0$ plane and the other around the $k_z=\pi/c$ plane along $<001>$. The latter type contributes to transport [23,24]. We calculated the quantum oscillation periods for both electron and hole pockets with the magnetic field applied both parallel and perpendicular to $<001>$ as a function of the hypothetical position of $\mu_0$. The DFT calculation accuracy is limited to several meV, making a perfect fit of all experimental oscillation frequencies with all calculations unrealistic. A $\mu_0=-8.2\pm0.7$ meV value range satisfies most of the observed oscillations (Fig. 4) and sets $\mu_0$ in the valence band, consistent with the positive thermopower observed at $T<25K$. The specific heat of the sample is analyzed (see supplement, Eq. S5 [15]) in terms of a linear electronic and a phonon term; the linear term has a coefficient $\gamma=1.5 \times 10^{-4}$ J/mol-K$^2$, comparing well with the calculated $\gamma=1.45 \times 10^{-4}$ J/mol-K$^2$ derived from the DOS at $\mu_0=-8.2$ meV.

The second parameter needed for quantitative comparison is scattering time $\tau$ assumed to be energy and temperature independent. DFT-derived values of $v_F\sim2\times10^5$ m s$^{-1}$ (confirmed by ARPES) and measured resistivity (see supplement [15]) yield $\tau\sim10^{-13}$ s.

The model (see supplement, Eq. S11 [15]) now can be compared to experimental data with all parameters determined independently of the Nernst and Seebeck measurements themselves. The calculated field and temperature dependences are reported in Figs. 2(b) and 3(b), showing exceptional agreement to experimental results, apart from the sign change theory predicts for the low-field Nernst effect below 40K. The amplitudes agree within a factor of 4, remarkable given the uncertainty of $\tau$. Fig. 3 shows in theory and experiment that the high-field Nernst coefficient peaks at $T_{MH} \approx \frac{\mu_0}{k_B}$, whereas near zero field, the Nernst coefficient peaks at $T_{ML} \approx \frac{3}{\pi} \frac{\mu_0}{k_B}$. The maximum at $T_{MS} \approx T_{ML}$, calculated for the Seebeck coefficient absolute value (Eq. 2), also is observed.

The model ignores trivial pockets in the Fermi surface by hypothesis, whereas band structure calculations valid in the 0K limit show they exist. When they are included in the Nernst and Seebeck effect calculations, the model diverges from experiment (see supplement [15]). We propose this as experimental evidence that non-Dirac bands do not contribute significantly to transport at temperatures above $\mu_0/k_B$. The behavior of $\alpha_{xxz}$ (Fig. 3(a) inset) strengthens this
argument. $\alpha_{x x z}$ tends to zero, a value reached rigorously in a Dirac band when $\mu(T) = 0$ (Eq. 2). If trivial pockets contributed to thermopower, $\alpha_{x x z}(T)$ would become metallic and increase monotonically with increasing temperature, as for Bi [10]. The partial thermopowers for the different trivial pockets of the Fermi surface that exist at low temperature can be inferred from the low temperature Fermi energies calculated for these pockets (see supplement [15]). If these pockets had been present at room temperatures, their partial thermopowers would have been of the order of 50-500 $\mu$V/K, compared to which the experimental value in Fig. 3a is factually zero. Because an accidental cancellation over a wide temperature range of the contributions of all non-Dirac bands is highly unlikely, we offer this as a reductio ad absurdum proof that the trivial pockets do not contribute. Furthermore, the near-perfect compensation between electron and hole pockets in the Dirac bands also explains the galvanomagnetic properties [2]. Although our analysis cannot identify the reason for this observation, the band structure temperature dependence might be responsible for this: most semiconductor band gaps increase (PbTe) or decrease (GaAs) by $\sim 100$ meV from cryogenic to room temperatures. Given the energy scale for Dirac fermions relevant to transport is an order of magnitude less, this may cause the disappearing trivial pocket importance with increasing temperature.

In conclusion, we experimentally and theoretically explored thermomagnetic transport in the inversion-symmetry-breaking WSM NbP. Two regimes in Nernst thermopower are seen: one for $H_z > |3T|$, and the other $H_z < |2T|$; both have non-monotonic temperature dependences. The theory explaining these properties quantitatively shows them to be Dirac band transport signatures, with no measurable contributions from trivial pockets above $\sim 100K$. Theory and experiment show that as the chemical potential shifts to the Dirac point energy with increasing temperature, the Nernst effect is maximized. At temperatures above the peak temperature, the Fermi function derivative broadens, leading states away from the Weyl nodes to contribute more to transport, lowering the Nernst thermopower and coefficient. The Nernst thermopower $\alpha_{y z z}(9T, 109K)$ exceeds 800 $\mu$V/K, surpassing the Seebeck thermopower $\alpha_{x x z}$ by two orders of magnitude. This study offers an understanding of the temperature dependence of the electrochemical potential position vis-à-vis the Weyl point and shows a direct connection between the Nernst effect and topology, a potentially robust mechanism for investigating topological states and the chiral anomaly.

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**FIGURE LABELS**

**Fig. 1:** Electrochemical potential band structure and motion with temperature. (a) Two-dimensional electronic dispersion relation (Eq. S6 in the supplement [15]) used in modeling NbP transport properties. (b) Two-dimensional dispersion around a single Dirac cone where, at low temperatures, the electrochemical potential lies in the valence band at an energy $\mu_0$ below the Dirac point. (c) Calculated $\mu(T)$ temperature dependence shows it moving towards the Weyl node energy with increasing temperature, from $|\mu_0|$, whether in the conduction or valence band. The energy scale is set to unity at $|\mu_0|$, and the temperature scale to unity at $|\mu_0/k_B|$.

**Fig. 2:** Nernst thermopower, $\alpha_{xyz}$ magnetic field dependence. (a) Measured Nernst thermopower as a function of applied magnetic field at various temperatures. The sharper slope for $|H|$ below $\sim 2T$ is the low-field regime; above $\sim 3T$ is the high-field regime. Systematic geometric error on the Nernst thermopower field dependence is $\sim 17\%$. Data are not symmetrized. Inset shows the Nernst voltage magnetic field dependence measured at 4.92K in a 2.17 mK temperature gradient. SDH oscillations are visible and correspond to DHVA periods measured in the magnetization. (b) Calculated at select temperatures, Nernst thermopower magnetic-field dependence given in SI and natural units that correspond well experimentally. The magnetic field is the product of the in-plane lattice constant $a$ and magnetic length $L_B \equiv \sqrt{\hbar c / eB}$; thermopower is $k_B/e$, and temperature in given units of $|\mu_0/k_B|$.

**Fig. 3:** Nernst coefficient, $N_{xyz}$ temperature dependence. (a) Measured Nernst coefficient plotted as a function of temperature (low-field regime in red, high-field in blue). The Nernst coefficient peaks near 50K (low-field) and 90K (high-field). Inset shows conventional thermopower temperature dependence, with a maximum near 8 $\mu$V/K, over two orders of magnitude smaller than the maximum Nernst thermopower. No magneto-thermopower is observed when a 9T magnetic field is applied parallel to the $\langle 001 \rangle$ axis. Error bars represent a 95% confidence interval on the systematic error standard deviation, excluding geometric error on the sample mount. (b) Calculated temperature dependence of the Nernst coefficient in the low-field (red) and high-field (blue) regimes. The given SI and natural units correspond very well without fitting.

**Fig. 4:** Electrochemical potential at 0K from DHVA periods and DFT calculations. Calculated (data points) and experimental (horizontal lines) values of the DHVA oscillation periods are
shown as a function of $\mu_0$ in the 0K limit, as measured from the W2 Dirac point. The $\mu_0 = -8.2 \pm 0.7$ meV values are represented by the hatched region, with the best overall fit in that box.

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Nernst coefficient; a theoretical analysis of effects of multiple Weyl nodes and trivial pockets; and plots of the analytical formulae in the main text.

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Fig. 2
Fig. 3
\[ H \perp <001> \]

\[ H \parallel <001> \]

\[ \mu_0 (\text{meV}) \]

\[ \text{dHvA periods (T)} \]

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