

**Emergent heat highways in the Weyl semimetal NdAlSi**

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Magnetic Weyl semimetals have emerged as a fertile ground for exploring quantum phases of matter and quasiparticles. The latter includes unconventional fermions with larger Chern numbers than those of conventional Weyl fermions and topologically nontrivial band structures in bosonic excitations. They hold potential for further experimental exploration of emergent quantum matter, magnon-polarons, which arise from hybridization between spin and lattice degrees of freedom. Such hybridization of distinct collective modes offers a pathway to control coupled degrees of freedom as well as quantum phases. Magnon-polarons are anticipated to mark their presence in heat transport. In our findings, we observed a significant rise in magnetothermal conductivity of the Weyl semimetal NdAlSi with complex magnetic order and a ferrimagnetic ground state. Furthermore, our theoretical results predict the existence of chiral phonons with nonvanishing pseudoangular momentum. Eventually, the huge increase in magnetothermal conductivity is attributed to the hybridization or strong coupling of magnons and chiral phonons. These charge-neutral excitations can drive significant advancements in the fields of magnonics, spintronics, and emerging topological quantum computing.

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**Introduction.** The interplay among magnetism, band topology, and electronic correlations plays a paramount role in enriching the quantum phenomena of topological materials. These include the observation of helical spin ordering driven by Weyl-mediated Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [1], the impact of magnetic orders on Weyl point regulation [2], and the emergence of quantum oscillations due to strong  $4f$ -electron exchange interaction [3]. Furthermore, the materials with broken-inversion and/or time-reversal symmetries are expected to host topological nontrivial characteristics not only in electronic [4] but also in phononic [5,6] and magnonic excitations spectra [7,8]. As a result, anomalous signatures in physical properties have been observed due to the quantum phenomena, namely, chiral and mixed axial-gravitational anomalies [9] and the thermal Hall effect because of the Berry phase associated with topological magnons [10] and phonons [5,11]. The interaction

between distinct degrees of freedom is of particular interest and has garnered significant attention in the field of condensed matter physics [12–14]. Moreover, the hybridization between magnons and phonons can harbor an emergent quantum matter called magnon-polaron [14–18]. Owing to the mixed characteristics of magnons and phonons, the dynamics of magnon-polarons could be regulated by external stimuli [19]. A comprehensive understanding and control of these collective magnetic excitations, magnon-polarons, is crucial for their potential applications in the fields of magnonics and spintronics. Although some efforts have been made to discover magnon-polarons [20,21], their signatures await experimental exploitation through thermal transport coefficients in magnetic Weyl semimetals. These charge-neutral excitations have been evaded by electrical transport and hence open the possibility of exploring their experimental characteristics in heat transport, as they are expected to offer a collective path for heat transfer [16,22–24]. For instance, thermal conductivity measurements offer a unique experimental approach for unfolding the emerging low-energy excitations in topological materials [25–27].

Recently, NdAlSi has been characterized as a magnetic type-II Weyl semimetal in which Weyl nodes are found to be regulated by the magnetic ordering [1,2]. The magnetic rich phase diagram of NdAlSi has been studied in detail by using neutron diffraction [1] and transport measurements under an applied magnetic field  $\mathbf{B} \parallel c$  [1,3,28]. At low temperatures,

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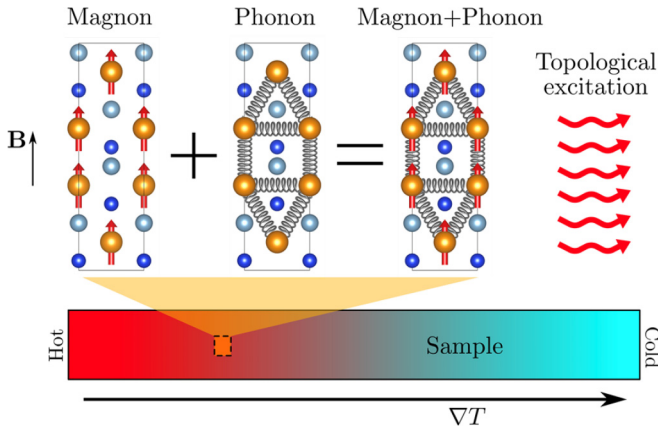


FIG. 1. Schematic coupling between magnon and phonon in NdAlSi. Unit cell of NdAlSi (in  $a$ - $c$  plane), wherein Nd, Al, and Si atoms are shown orange, light blue, and blue, respectively. Magnons arise from the interplay between the magnetic moments (red arrows) of Nd atoms. Similarly, phonons, representing lattice vibrations, result from the elastic arrangement of atoms, illustrated by springs (showing only the interactions between Nd atoms). In the field-induced ferromagnetic phase, phonon-magnon coupling leads to the formation of hybrid-collective excitation that can carry heat when subjected to external heat stimuli.

spin-density-wave order is realized with the lack of magnetic field, and it can be destroyed by applying a sufficiently strong external magnetic field [1]. Additionally, the simultaneous presence of magnons and chiral phonons provides the possibility of the emergence of magnon-polarons in NdAlSi (see schematic Fig. 1). They hold great promise for technological applications in spintronics and quantum information, as they are less prone to Joule heating and can be tuned by an external magnetic field [7,8,19].

Here, we employed electric (and thermal) transport measurements on single-crystalline NdAlSi; an electric (and heat) current was applied along the  $a$  axis under a magnetic field  $B$  oriented along the  $c$  axis. The positive magnetoresistance (MR) was observed at various temperatures. Surprisingly, a huge increase in thermal conductivity was noticed at low temperatures in high magnetic field (ranging from 6 to 14.5 T), demonstrating the potential use as a solid-state thermal switch [29]. Our theoretical results predicted the existence of circularly polarized/chiral phonons even though NdAlSi does not belong to the chiral group. In NdAlSi, the absence of a symmetry center leads to the formation of chiral phonons, which are mostly associated with the circular motion of Nd ions around the equilibrium position. As a result, these phonons are anticipated to have strong coupling with magnons [30]. Furthermore, based on a comprehensive analysis, we concluded that the observed increase in thermal conductivity cannot be solely explained by electronic, phononic, and magnonic contributions. Instead, the phenomenon was attributed to the synergy of magnons and chiral phonons, resulting in magnon-polaron formation.

**Results and discussion.** Figure 2 represents the isothermal magnetoresistivity  $\rho(B)$  of NdAlSi measured under applied magnetic field  $B \parallel c$  and  $I \parallel a$ . Observed steplike anomalies in  $\rho(B)$ , see magenta arrow in Fig. 2, are caused by the

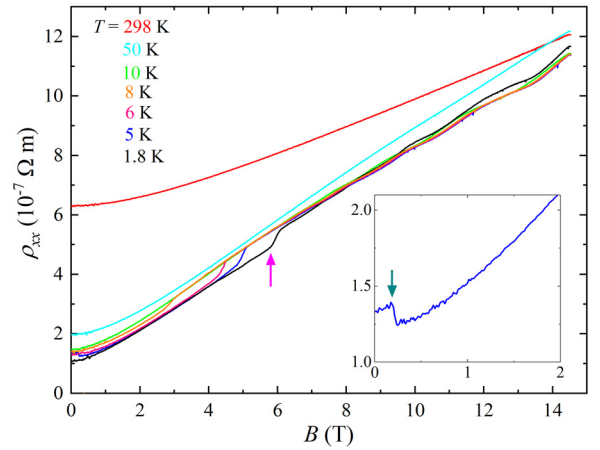


FIG. 2. Isothermal magnetoresistivity [ $\rho_{xx}$ ] of NdAlSi.  $\rho_{xx}$  measured with the electric current applied along the  $a$  axis and magnetic field oriented along the  $c$  axis. Steplike dips (inset) and jumps are shown by the dark cyan and magenta arrows.

disappearance of the spin-density wave vector [1]. As a result, there is a sudden increase in carrier density [28], and the gap between nested parts of the Fermi surface vanishes. This affects the transport properties and leads to such anomalies [1,3,28]. In the low-magnetic-field regime, a steplike dip is observed in  $\rho(B)$  around  $T \approx 5$  K (as shown in the inset of Fig. 2). This dip is related to metamagnetic (spin-flip) transitions induced by the external magnetic field along the easy axis [3]. The positions of this magnetic transition are in good agreement with previous reports [3,28]. At low temperatures,  $\rho(B)$  shows quantum oscillations (refer to Fig. S1 in the Supplemental Material (SM) [31]), with frequencies consistent with previous reports [1,3,28]. For all temperatures,  $\rho(B)$  increases and shows no sign of saturation up to  $B = 14.5$  T. This large positive MR can be expected for a Weyl semimetal as found in an earlier report [32].

Figure 3 depicts the temperature dependence of thermal conductivity  $\kappa$  at constant magnetic fields  $B = 0, 5, 10$ , and  $14.5$  T and comparison of  $\kappa$  with the zero-field electronic thermal conductivity calculated from  $\rho$  using the Wiedemann-Franz (WF) law  $\kappa_{WF} = \sigma L_0 T$ , where  $L_0$  is the Sommerfeld value of the Lorenz number for free electrons. Here,  $\kappa(T)$  passes through a maximum value at  $T \approx 60$  K while cooling down from room temperature. At this temperature, phonons account for  $\sim 73\%$  of the total thermal conductivity. Later,  $\kappa(T)$  decreases over the temperature range from 60 to 10 K. Notably, at 10 K,  $\kappa_{WF}$  appears to make a significant contribution to the total thermal conductivity. Below 10 K,  $\kappa(T)$  begins to rise again, reaching a maximum at 5 K (see blue curve in the inset of Fig. S3 in the SM [31]), indicating the emergence of magnons and their role in thermal conduction. In fact, such a peak is observed in magnetic materials below the Neel temperature  $T_N$ , as a characteristic feature of magnon contribution, which can account for a significant portion of total thermal conductivity [33]. The inset of Fig. 3 depicts the further comparison of  $\kappa_{WF}(T)$ , in zero field, with  $\kappa(T)$  at various constant fields for  $T \leq 20$  K. First, for  $T \leq 10$  K,  $\kappa(T)$  decreases with increasing the constant magnetic field, reaching a critical magnetic field  $B_{C1}$ , which

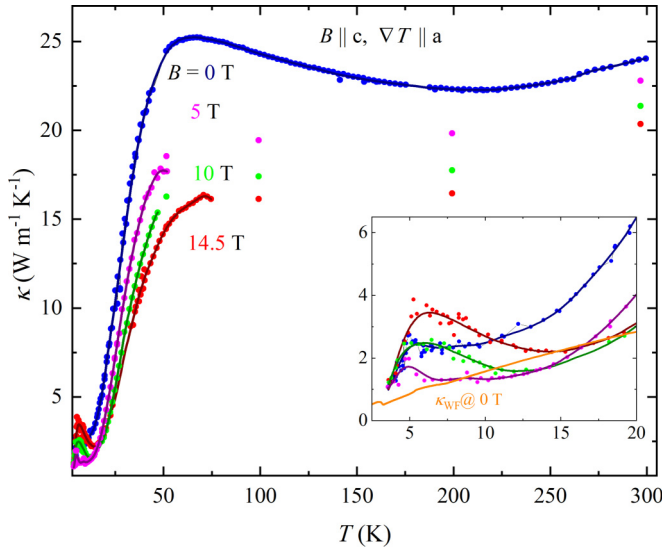


FIG. 3. Temperature dependence of the  $a$ -axis thermal conductivity for NdAlSi at constant magnetic field ( $B$ ).  $\kappa(T)$  data are plotted with blue, pink, green, and red points at  $B = 0, 5, 10$ , and  $14.5$  T, respectively. The inset shows a zoomed-in plot of  $\kappa(T)$  along with the electronic contribution  $\kappa_{WF}(T)$  (orange line) calculated using the Wiedemann-Franz law. At low temperatures,  $\kappa(T)$  attained a maximum value at magnetic-field-transition temperature that can be viewed as a fingerprint of magnons involvement in thermal conduction, which decreases with increasing the constant field and eventually turns out to broad peaks in high  $B$ .

also correlates with the crossover from ferrimagnetic to a field-induced ferromagnetic state [3,28]. Such a crossover can also be realized through the suppression of the lambda-point anomaly in specific heat, indicating long-range magnetic ordering [34], by an external magnetic field [3]. Remarkably, beyond  $B_{C1}$ ,  $\kappa(T)$  starts to rise with an increasing constant magnetic field.

Figures 4(a) and 4(b) present the magnetic field dependences of  $\kappa_{WF}$  and  $\kappa$  at low temperatures ( $T \leq 10.7$  K), respectively. As shown in Fig. 4(a),  $\kappa_{WF}$  decreases with

the visible anomalies as the magnetic field increases, which is a consequence of MR. Below 5 K, magnetothermal conductivity  $\kappa(B)$  initially increases up to  $B_c \approx 3$  T and, afterward, starts to decline until reaching  $B_{C1}$ . This reduction of  $\kappa(B)$  persists up to high temperatures, exhibiting the anomalies at  $B_{C1}$ . In the high-field limit,  $\kappa(B)$  increases at low temperatures. At low temperatures, charge carriers (electrons or/and holes) are the primary contributors to thermal conductivity in the absence of the magnetic field. However, their contribution decreases markedly in the magnetic field. This indicates that electronic thermal conductivity is unlikely to be responsible for the enhancement of total magnetothermal conductivity within high-field limits. Previously, a substantial increase in  $\kappa(B)$  was ascribed to a gravitation anomaly in Weyl semimetals [35,36]. The gravitation anomaly is highly sensitive to field orientation like the chiral anomaly [37] and only emerges in the presence of a collinear temperature gradient  $\nabla T$  and magnetic field in the direction of Weyl point separation. However, the contribution of the mixed axial-gravitational anomaly to the experimentally measured longitudinal thermal conductivity can be observed at angles of a few degrees due to a slight misalignment between the magnetic field and  $\nabla T$ . When the magnetic field is oriented perpendicular to  $\nabla T$ , there is no observed contribution from the mixed axial-gravitational anomaly to thermal conduction. Therefore, the observed increase in this configuration (when  $\nabla T$  is perpendicular to  $B$ ) is unlikely to be attributed to electronic or mixed axial-gravitational contribution. Moreover, we observed a drastic violation of the WF law in the field-induced ferromagnetic phase at various temperatures [shown in Figs. 4(a) and 4(b)]. Generally, the WF law is expected to hold at low and high temperatures (in the case of NdAlSi, at room temperature, see Fig. S2 in the Supplemental Material [31]) if charge carriers scatter elastically, resulting in equal degradation of charge and heat currents. However, the emergence of new chargeless heat pathways contributes to a significant violation of the WF law, for instance, in the case of the chiral zero sound, which creates an additional chargeless heat conduction channel, leading to a severe violation of the WF law [25,26].

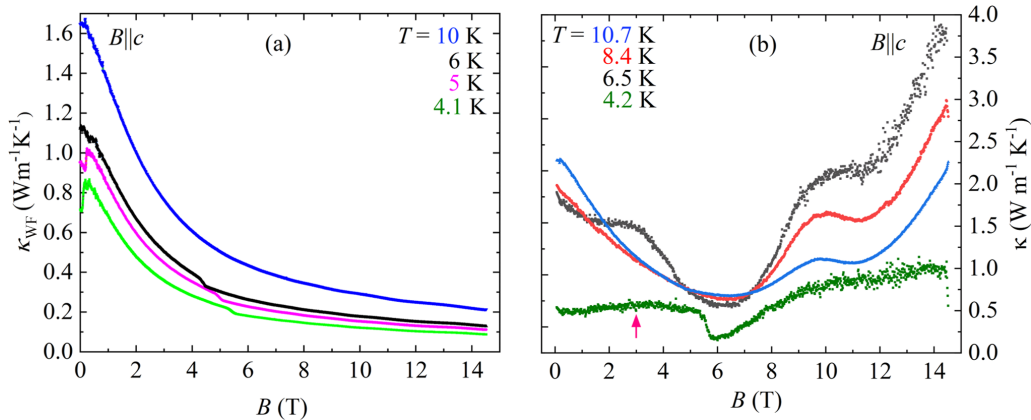


FIG. 4. Magnetic field dependence of thermal conductivity of NdAlSi. (a) Electronic thermal conductivity  $\kappa_{WF}(B)$  at  $T = 4.1, 5, 6$ , and  $10$  K (bottom to top), calculated using the WF law. (b) Total thermal conductivity measured at  $T = 4.2, 6.5, 8.4$ , and  $10.7$  K. The pink arrow represents  $B_c$  at  $T = 4.2$  K (green curve).

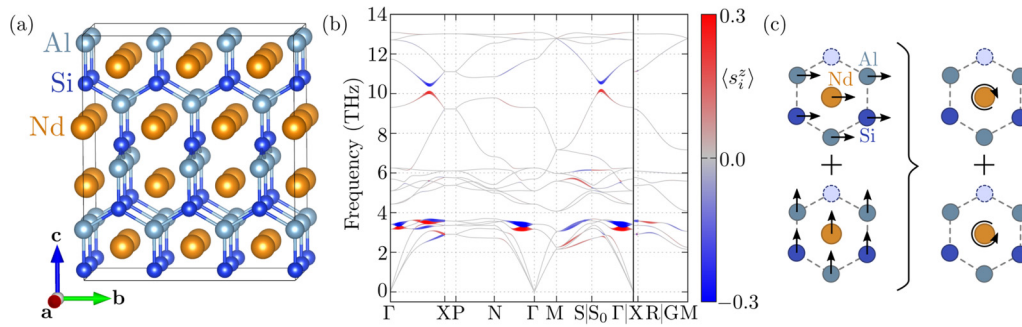


FIG. 5. Crystal structure and lattice dynamic of NdAlSi. (a) Crystal structure of NdAlSi and characteristic zig-zag chains formed by Al and Si atoms along  $a$  and  $b$  directions. Elementary lego block of NdAlSi is formed by the imperfect hexagonal-like cages build by Al and Si atoms. One Nd atom is located inside each cage. (b) Phonon dispersion curves exhibit nonvanishing total pseudoangular momentum (PAM), here presented by the color line. The phonon branches possess nonzero PAM outside of the high-symmetry points, due to the absence of the inversion symmetry. (c) Acoustic modes at the  $\Gamma$  point are related to the zero-frequency  $E$  mode (movement of all atoms along  $a$  or  $b$  directions) and zero-frequency  $A$  mode (movement of all atoms along the  $c$  direction). Outside of  $\Gamma$ , the phonon branches correspond to chiral phonons formed by the combination of the mentioned modes. Such chiral phonons are mostly related to the circular motion of the Nd atom around the equilibrium position.

Since NdAlSi is a magnetic Weyl semimetal, it is worth investigating the extent to which lattice and magnonic thermal conductivities account for the total thermal conductivity at low temperatures. The former was found to be an order smaller than the total thermal conductivity (see Fig. S3 in the SM [31]), independently calculated using the specific heat of nonmagnetic sister material LaAlSi and  $\kappa$  (described in a previous report [36]). Moreover, the phonon contribution may be affected by two phenomena in the magnetic field. First, it might be attenuated by the magnons below  $T_N$  [38] and expected to recover in the magnetic field as the scattering of phonons over magnons/magnetic defects are supposed to be reduced. Secondly, the phonon-phonon scattering increases due to the anharmonic motion of lattice [39]. Additionally, in NdAlSi, the crystal-electric-field (CEF) splits the tenfold-degenerate  $j$  multiplet of  $\text{Nd}^{3+}$  into a ground-state doublet and four degenerate excited doublets [1]. Their characteristics are observable in specific heat as a broad hump known as the Schottky anomaly. The phonon scatters off the CEF multiplets in a way that, first, a phonon of energy matching the CEF split levels is absorbed and then emitted with the same energy but with different momentum. Such phonon-resonant scattering limits the phonon heat conduction [40]. Nonetheless, it was observed that these competitive phenomena resulted in a slight increase in magnetothermal conductivity [41–43]. We also observed such a small increase of  $\kappa(B)$  at  $T \sim 20$  K (Fig. S4 in the SM [31]). On the other hand, at low temperatures, we observed a remarkable increase of  $\kappa(B)$  in the field-induced ferromagnetic phase (see the region above the black dots added as a guide to the eye, Fig. S5 in the SM [31]). Given that, one can conclude that such an increase appears not to be solely related to the phononic contribution.

Finally, in magnetic materials, magnons carry heat in two ways: either they themselves contribute to thermal conductivity or hybridize with phonons at anticrossing region points, forming a collective/coupled magnetoelastic mode (to be discussed). However, the application of a sufficiently large magnetic field creates a gap (the minimum energy required for propagating the magnons) in the density of state (DOS)

for magnons, i.e., a gap smaller than the Zeeman energy. Thus, the magnon contribution was found to be frozen out in the specific heat capacity [3] in the presence of the magnetic field. Nevertheless, the magnon contribution to total thermal conductivity is expected to diminish exponentially with increasing magnetic field [44]. Therefore, magnons carry negligibly small additional heat in the field-induced ferromagnetic phase due to an opening of the magnetic-excitation gap [22], and the energy corresponding to the temperature, i.e., thermal activation energy, is not comparable with the gap energy, calculated using specific heat capacity [3]. Moreover, this magnetic-excitation gap appears to merge in a low field [3], resulting in a slight increase in  $\kappa(B)$  [45] up to  $B_c \approx 3$  T, particularly at  $T \approx 4.2$  K. Apparently, in the high-field limit, this substantial increase of  $\kappa(B)$  also cannot be attributed to the magnon contribution.

After considering all possible contributions to  $\kappa(B)$ , let us focus now on the lattice dynamics of NdAlSi. The crystal structure contains the zig-zag-like chains of Al-Si atoms, arranged alternately along  $a$  and  $b$  directions [Fig. 5(a)]. From this, an elementary lego block is formed by the imperfect hexagonal-like cage build by Al and Si atoms. Inside each cage, there is only one Nd atom. The surprising result of the interplay between the Nd atom with surrounding Al-Si environment can lead to formation of the chiral phonons with nonzero total pseudoangular momentum (PAM) outside the high-symmetry points of the Brillouin zone [Fig. 5(b)]. Indeed, analysis of the phonon circular polarization for each atom uncovers the manifested chiral phonons (see Figs. S6 and S7 in the SM [31]). Moreover, each atom in the structure can lead to chiral phonons but at different ranges of frequencies (see Fig. S7 in the SM [31]). Similar behavior was earlier reported for the magnetic topological insulators  $\text{TBi}_2\text{Te}_4$  ( $T = \text{Fe}$  and  $\text{Mn}$ ) [46]. However, the presence of inversion symmetry causes the total PAM of phonons to vanish. Here, the absence of inversion symmetry [6] makes it possible to have a nonzero total PAM in some phonon branches. The chiral phonons, away from the high-symmetry points, can be understood as a combination of the vibration modes at the

$\Gamma$  point. For example, the acoustic modes at the  $\Gamma$  point are related to the movement of all atoms along the  $a$  or  $b$  direction (zero-frequency mode with  $E$  symmetry) and the movement along the  $c$  direction (zero-frequency mode with  $A$  symmetry), presented schematically in Fig. 5(c). Here, dashed circles correspond to the missing Al or Si atom in the earlier mentioned cagelike structure formed by the Al-Si honeycomblike lattice. This clearly shows the breaking of inversion symmetry in two ways: first, because of the existence of two types of atoms in a honeycomblike lattice and, second, because of the absence of one atom in such a structure.

The realization of chiral phonons does not depend on the magnetic order but directly on the system symmetry. Moreover, typically, chiral phonons are expected in a system with threefold rotational symmetry, e.g., hexagonal systems like a honeycomb lattice [47]. Nevertheless, also, local symmetry can play a role in forming chiral phonons. For example, ABi ( $A = \text{K, Rb, and Cs}$ ) with monoclinic  $P2_1/c$  symmetry possesses chiral phonons within the chains with locally threefold rotational symmetry [48]. Similarly, in our case, independently from the tetragonal  $I4_1md$  symmetry, the interplay between Nd with neighboring Al and Si atoms leads to chiral phonons. Additionally, the external magnetic field can lead to enhancement of the circular polarization due to effective orbital moment [49]. For example, the double-degenerated  $E$ -like modes at the  $\Gamma$  point can be decoupled into two modes with opposite circulations. Such an effect was observed experimentally in  $\text{CeF}_3$ , within Raman scattering measurements [50]. This is possible due to the interplay between the phonon angular momentum with the magnetic field [51].

Interplay between (chiral) acoustic phonons and magnons can be crucial in the range of low-temperature limits. At relatively high temperatures, the phonon thermal conductivity in practice is related to the whole phonon spectrum. In such a situation, the phonon lifetime  $\tau_q^{pp}$  is comparable for all phonon branches. However, with decreasing temperature, the role of low-frequency phonon branches is more important. This directly enhances the phonon lifetime for low frequencies (see Fig. S8 in the SM [31]). Moreover, assuming only phonon-phonon scatterings, the thermal conductivity diverges with  $T \rightarrow 0$ . The scattering due to the boundary can be introduced using Matthiessen's rule  $\frac{1}{\tau_q^{\text{total}}} = \frac{1}{\tau_q^{pp}} + \frac{2|v_q|}{L}$ , where the second term denotes the scattering rate due to a grain boundary of size  $L$  (sample size) which depends on the phonon group velocity  $v_q$ . Theoretically obtained thermal conductivity is overestimated by a few magnitudes. Nevertheless, it shows that the results do not depend on the assumed magnetic order (see Fig. S9 in the SM [31]). However, theoretical results do not consider the magnon-phonon scattering process as well as the interplay of chiral phonons with magnetic fields.

An important question is to what extent the interplay between chiral phonon and magnon affects the measured total thermal conductivity at various temperatures in the magnetic field. Moreover, materials with sizable Dzyaloshinskii-Moriya interaction (DMI) may host topological magnons [7]. Magnons with nontrivial bands are rarely realized in real material, as they are not allowed by certain symmetries [7]. Nevertheless, it is not necessary to have either chiral phonons or topological magnons for their hybridization. However, the existence of chiral phonons strengthens the possibility of

their strong coupling with magnons [30]. Moreover, at low temperatures, the simultaneous presence of chiral acoustic phonons and magnon can lead to magnon-phonon hybridization at the avoided crossing of magnon and phonon bands, resulting in coherent hybridization modes [23,52]. In NdAlSi, the lack of a symmetry center results in phonons with nonzero PAM, which hybridize with magnons to form magnon-polaron excitations. More specifically, due to the hybridization between magnon and phonon bands, a gap opens at the avoided crossing. In addition, the inversion of the bands takes place between magnons and phonons [14]. As a result, the bands acquire the hybrid signature of the magnonic and phononic characteristics.

For example, magnon-polarons are considered low-energy excitations, so-called Goldstone modes [53]. Magnon-polarons are considered elementary excitations and predicted to emerge in a magnetic field [52,54]. Alternatively, the phonon band turns out to be tangent to the magnon band while increasing magnetic field [21]. Altogether, they are supposed to carry heat when subjected to external heat stimuli. Moreover, the hybridized phonon and magnon bands have Berry curvature in the anticross region points (or act as hotspots of Berry curvature). Therefore, these hybrid bands have nonzero Chern numbers and are considered topologically nontrivial, and we refer to these hybrid modes as topological magnon-polarons. The magnon-polaron can be used to modulate the magnon dynamics [23]. The interaction between phonons and magnons is facilitated by magnetoelastic coupling and DMI [14,23,24]. The experimental signatures of these phenomena are expected in spin and energy transport, specifically in thermal conductivity measurements [20,22]. For instance, the magnon-polaron is anticipated to give rise to anomalous peaks in the field dependence of the spin Seebeck effect [20,21]. These peaks manifest at the magnetic field values that correspond to the anticrossing points of the magnon and phonon dispersion curves. However, the positions of the magnon-polaron peaks may also be influenced by the degree of anisotropy present in the system. From a technological perspective, they can enhance the spin-pumping effect [55], allowing the generation and manipulation of spin currents through phonon involvement as phonons and magnons are hybridized.

This paves the way for the search of the coupling of magnons and chiral phonons in the magnetic Weyl semimetal NdAlSi. Our theoretical prediction further strengthens the presence of a magnon-polaron. We believe that, at low temperatures, in-field enhancement of thermal conductivity is related to this topological excitation—a topological magnon-polaron. The magnon-polaron creates additional heat conduction pathways that apparently violate the WF law.

As explained earlier, the nonzero Berry curvature arises from strong coupling or hybridization between magnons and phonons around the anticrossing of their dispersion curves [23]. The Berry curvature in this case is opposite to that associated with the pure magnon bands [22]. As a result, a sign reversal of the thermal Hall coefficient (THC) is expected along with the substantial increase in longitudinal thermal conductivity [22,23]. Such a characteristic has been observed in NdAlSi, namely, the positive THC in the low-field

region and negative THC in the field-induced ferromagnetic phase [56].

Interestingly, the nonmonotonic increase in  $\kappa(B)$  displays an anomaly, forming a valley [see Fig. 4(b)]. This observed phenomenon could be due to spin fluctuations within the crossover regions [57,58]. These fluctuations might lead to (anti)crossings of phonon and magnon spectra in a complex manner or even cause these spectra to become more distant. Consequently, our results emphasize the need for further experimental (inelastic scattering spectroscopy) and theoretical insights into the coupling between phonons and magnons, including their cross/anticross behavior and the dynamics of magnon-polarons in the presence of an external magnetic field.

**Conclusions.** In summary, magnetoelectrical and magnetothermal transport was performed in Weyl semimetal NdAlSi. At low temperatures and in low magnetic fields, magnons carry a significant amount of heat, and their contribution to total thermal conductivity is suppressed by increasing the magnetic field. In the field-induced ferromagnetic phase, the observed huge increase in magnetothermal conductivities was related to the topological magnon-polaron, emerging from the hybridization of the chiral acoustic phonons with the magnons. These topological excitations carry heat in the presence of a magnetic field, suggesting an important role for chiral phonons in heat transport. In our study, we not only shed light on the fundamental aspects of the phonon-magnon interplay but also open the door to technological applications since thermal conductivity can be substantially modulated by a magnetic field.

**Methods: Experimental details.** Single crystals of NdAlSi were grown by a self-flux, and the related insightful information was reported in the previous report [1]. NdAlSi has a noncentrosymmetric centered tetragonal crystal structure  $I4_1md$  (space group No. 109), with lattice constants  $a = b = 4.201 \text{ \AA}$  and  $c = 14.516 \text{ \AA}$  [3]. The single crystals of NdAlSi were grown to be longer along the  $a$  axis [1]. For the transport measurements, a rectangular bar with dimensions  $1.9 \times 1.4 \times 0.35 \text{ mm}^3$  was cut from a suitable single crystal with the longest side of the sample oriented along the [100] direction (crystallographic  $a$  axis that is a magnetic hard axis) and the shortest side along the [001] direction (crystallographic  $c$  axis that is an easy axis). The electrical measurements were performed using a standard four-point technique with an alternating electric current applied along [100] in the temperature  $T$  range 1.8–300 K. The contacts were made with Ag paste over the cross-section surface to maintain the uniform current flow. The magnetic field  $B$  was applied up to 14.5 T, perpendicular to the electric current  $B \parallel c$ . Field sweeps up and down are utilized to extract the symmetric components of  $\sigma(B)$  and  $\kappa(B)$ .

Thermal conductivity ( $\kappa$ ) measurements were done using the isolated heater method, detailed in Ref. [26]. In thermal conductivity measurement, two contacts with Ag wire were made across the sample and then connected with a Chromel-Constantan thermocouple. The sensitivity of type- $E$  thermocouples decreases as the temperature lowers, resulting in a noisier signal in the low-temperature region. This type of thermocouple exhibits a field dependency that re-

quires correction. In our study, we considered their in-field calibration. The thermocouples were calibrated with the help of a Cernox chip, whose sensitivity shows a weak magnetic field dependency. During measurements, the thermal gradient  $\nabla T$  was applied along the  $a$  axis, and the magnetic field was perpendicular to the thermal gradient, i.e., along the  $c$  axis like the electrical measurements. At low temperatures, we paid special attention to the operation of the resistive heater. We supplied power in such a way that the temperature difference ( $\Delta T$ ) remained  $<10\%$  of the sample temperatures. Additionally, we employed an additional thermocouple and a Cernox chip (placed at the heat sink) to measure the mean temperature of the sample during the measurements.

**Methods: First-principles calculations.** The first-principles density functional theory (DFT) calculations were performed using the projector augmented-wave potentials [59] implemented in the VASP code [60–62]. For the exchange-correlation energy, the generalized gradient approximation in the Perdew, Burke, and Ernzerhof parametrization was utilized [63]. Comprehensive details on the calculations (first-principles, lattice dynamics, and chiral phonons) are included in Notes S6 and S7 in the SM [31].

**Methods: Error analysis.** The absolute measurement error in thermal conductivity is mainly dominated by sample geometrical factor measurement uncertainty ( $\sim 10\%$ ) due to the finite size of voltage/thermal gradient contacts. Despite that, we have considered all possible heat losses, not only radiation but also heat loss by conduction and heat loss by diffusion. We tried to minimize them. For example, the heat loss by conduction is minimized using thin and long wire thermocouples. To do so, we make them in coil form. The heat loss by diffusion was minimized by placing the brass can to keep the probe under the vacuum throughout the measurement. We have succeeded in doing so, as no pressure disturbance is observed during the entire set of measurements. Finally, radiation heat losses are minimized by placing a silver radiation shield over the setup. An additional sample heater was placed on the surface of the radiation shield. The heater is mounted to face the sample heater, and the same current was applied to both heaters to achieve thermal equilibrium or minimize the temperature difference between them. Furthermore, radiation heat losses are negligible in the low-temperature regime (see Fig. S10 in the SM [31]). Nevertheless, we considered the radiation losses while analyzing the thermal conductivity.

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P.K.T. and M.M. conducted the experiment and performed the respective analyses. S.Y. and A.P. performed the

theoretical part. P.K.T., S.Y., A.P., and M.M. prepared the initial version of the manuscript. X.Y. and F.T. prepared the single crystals. All authors helped in reviewing, editing, and discussing the results as well as participated in writing the manuscript.

The authors declare no competing financial interests.

**Data Availability.** The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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- [1] J. Gaudet, H. Y. Yang, S. Baidya, B. Lu, G. Xu, Y. Zhao, J. A. Rodriguez-Rivera, C. M. Hoffman, D. E. Graf, D. H. Torchinsky *et al.*, Weyl-mediated helical magnetism in NdAlSi, *Nat. Mater.* **20**, 1650 (2021).
- [2] C. Li, J. Zhang, Y. Wang, H. Liu, Q. Guo, E. Rienks, W. Chen, F. Bertran, H. Yang, D. Phuyal *et al.*, Emergence of Weyl fermions by ferrimagnetism in a noncentrosymmetric magnetic Weyl semimetal, *Nat. Commun.* **14**, 7185 (2023).
- [3] J.-F. Wang, Q.-X. Dong, Y.-F. Huang, Z.-S. Wang, Z.-P. Guo, Z.-J. Wang, Z.-A. Ren, G. Li, P.-J. Sun, X. Dai *et al.*, Quantum oscillations in the magnetic Weyl semimetal NdAlSi arising from strong Weyl fermion- $4f$  electron exchange interaction, *Phys. Rev. B* **108**, 024423 (2023).
- [4] 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 *et al.*, Experimental discovery of Weyl semimetal TaAs, *Phys. Rev. X* **5**, 031013 (2015).
- [5] T. Qin, J. Zhou, and J. Shi, Berry curvature and the phonon Hall effect, *Phys. Rev. B* **86**, 104305 (2012).
- [6] S. Coh, Classification of materials with phonon angular momentum and microscopic origin of angular momentum, *Phys. Rev. B* **108**, 134307 (2023).
- [7] F.-Y. Li, Y.-D. Li, Y. B. Kim, L. Balents, Y. Yu, and G. Chen, Weyl magnons in breathing pyrochlore antiferromagnets, *Nat. Commun.* **7**, 12691 (2016).
- [8] A. Mook, J. Henk, and I. Mertig, Tunable magnon Weyl points in ferromagnetic pyrochlores, *Phys. Rev. Lett.* **117**, 157204 (2016).
- [9] J. Gooth, A. C. Niemann, A. G. Grushin, T. Meng, K. Landsteiner, B. Gotsmann, F. Menges, M. Schmidt, C. Shekhar, V. Süß *et al.*, Experimental signatures of the mixed axial-gravitational anomaly in the Weyl semimetal NbP, *Nature* **547**, 324 (2017).
- [10] Y. Onose, T. Ideue, H. Katsura, Y. Shiomi, N. Nagaosa, and Y. Tokura, Observation of the magnon Hall effect, *Science* **329**, 297 (2010).
- [11] G. Grissonnanche, S. Thériault, A. Gourgout, M.-E. Boulanger, E. Lefrançois, A. Ataei, F. Laliberté, M. Dion, J.-S. Zhou, S. Pyon *et al.*, Chiral phonons in the pseudogap phase of cuprates, *Nat. Phys.* **16**, 1108 (2020).
- [12] Z. Zhang, F. Y. Gao, J. B. Curtis, Z.-J. Liu, Y.-C. Chien, A. von Hoegen, M. T. Wong, T. Kurihara, T. Suemoto, P. Narang *et al.*, Terahertz field-induced nonlinear coupling of two magnon modes in an antiferromagnet, *Nat. Phys.* **20**, 801 (2024).
- [13] T. W. J. Metzger, K. A. Grishunin, C. Reinhofer, R. M. Dubrovín, A. Arshad, I. Ilyakov, T. V. A. G. de Oliveira, A. Ponomaryov, J.-C. Deinert, S. Kovalev *et al.*, Magnon-phonon Fermi resonance in antiferromagnetic CoF<sub>2</sub>, *Nat. Commun.* **15**, 5472 (2024).
- [14] S. Bao, Z.-L. Gu, Y. Shangguan, Z. Huang, J. Liao, X. Zhao, B. Zhang, Z.-Y. Dong, W. Wang, R. Kajimoto *et al.*, Direct observation of topological magnon polarons in a multiferroic material, *Nat. Commun.* **14**, 6093 (2023).
- [15] A. Kamra, H. Keshtgar, P. Yan, and G. E. W. Bauer, Coherent elastic excitation of spin waves, *Phys. Rev. B* **91**, 104409 (2015).
- [16] K. Shen and G. E. W. Bauer, Laser-induced spatiotemporal dynamics of magnetic films, *Phys. Rev. Lett.* **115**, 197201 (2015).
- [17] E. Thingstad, A. Kamra, A. Brataas, and A. Sudbø, Chiral phonon transport induced by topological magnons, *Phys. Rev. Lett.* **122**, 107201 (2019).
- [18] D. A. Bozhko, P. Clausen, G. A. Melkov, V. S. L'vov, A. Pomyalov, V. I. Vasyuchka, A. V. Chumak, B. Hillebrands, and A. A. Serga, Bottleneck accumulation of hybrid magnetoelastic bosons, *Phys. Rev. Lett.* **118**, 237201 (2017).
- [19] J. N. Kløgetvedt and A. Qaiumzadeh, Tunable topological magnon-polaron states and intrinsic anomalous Hall phenomena in two-dimensional ferromagnetic insulators, *Phys. Rev. B* **108**, 224424 (2023).
- [20] B. Flebus, K. Shen, T. Kikkawa, K.-i. Uchida, Z. Qiu, E. Saitoh, R. A. Duine, and G. E. W. Bauer, Magnon-polaron transport in magnetic insulators, *Phys. Rev. B* **95**, 144420 (2017).
- [21] T. Kikkawa, K. Shen, B. Flebus, R. A. Duine, K. I. Uchida, Z. Y. Qiu, G. E. W. Bauer, and E. Saitoh, Magnon polarons in the spin Seebeck effect, *Phys. Rev. Lett.* **117**, 207203 (2016).
- [22] N. Li, R. R. Neumann, S. K. Guang, Q. Huang, J. Liu, K. Xia, X. Y. Yue, Y. Sun, Y. Y. Wang, Q. J. Li *et al.*, Magnon-polaron driven thermal Hall effect in a Heisenberg-Kitaev antiferromagnet, *Phys. Rev. B* **108**, L140402 (2023).
- [23] X. Zhang, Y. Zhang, S. Okamoto, and D. Xiao, Thermal Hall effect induced by magnon-phonon interactions, *Phys. Rev. Lett.* **123**, 167202 (2019).
- [24] J. Cui, E. V. Boström, M. Ozerov, F. Wu, Q. Jiang, J.-H. Chu, C. Li, F. Liu, X. Xu, A. Rubio *et al.*, Chirality selective magnon-phonon hybridization and magnon-induced chiral phonons in a layered zigzag antiferromagnet, *Nat. Commun.* **14**, 3396 (2023).
- [25] J. Xiang, S. Hu, Z. Song, M. Lv, J. Zhang, L. Zhao, W. Li, Z. Chen, S. Zhang, J.-T. Wang *et al.*, Giant magnetic quantum oscillations in the thermal conductivity of TaAs: Indications of chiral zero sound, *Phys. Rev. X* **9**, 031036 (2019).
- [26] P. K. Tanwar, M. S. Alam, M. Ahmad, D. Kaczorowski, and M. Matusiak, Severe violation of the Wiedemann-Franz law in quantum oscillations of NbP, *Phys. Rev. B* **106**, L041106 (2022).

- [27] P. Czajka, T. Gao, M. Hirschberger, P. Lampen-Kelley, A. Banerjee, J. Yan, D. G. Mandrus, S. E. Nagler, and N. P. Ong, Oscillations of the thermal conductivity in the spin-liquid state of  $\alpha$ -RuCl<sub>3</sub>, *Nat. Phys.* **17**, 915 (2021).
- [28] J.-F. Wang, Q.-X. Dong, Z.-P. Guo, M. Lv, Y.-F. Huang, J.-S. Xiang, Z.-A. Ren, Z.-J. Wang, P.-J. Sun, G. Li *et al.*, NdAlSi: A magnetic Weyl semimetal candidate with rich magnetic phases and atypical transport properties, *Phys. Rev. B* **105**, 144435 (2022).
- [29] K. G. Koster, J. Hise, J. P. Heremans, and J. E. Goldberger, Giant magnetothermal conductivity switching in semimetallic WSi<sub>2</sub> single crystals, *ACS Appl. Electron. Mater.* **6**, 1762 (2024).
- [30] J. Holanda, D. S. Maior, A. Azevedo, and S. M. Rezende, Detecting the phonon spin in magnon-phonon conversion experiments, *Nat. Phys.* **14**, 500 (2018).
- [31] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/yj5v-jymb> for data on quantum oscillation at various temperature; lattice thermal conductivity, magnetothermal conductivity at  $T = 20$  and  $34$  K; magnetic phase diagram constructed from thermal conductivity values; comprehensive details on first-principles calculations and lattice dynamics, including phonon dispersion and chiral polarization of each atom; phonon lifetime, temperature-dependent theoretically obtained phonon thermal conductivity for paramagnetic, antiferromagnetic, and ferromagnetic order; room-temperature thermal conductivity in the magnetic field; and radiation heat losses, which includes Refs. [28,47,64–69].
- [32] C. Shekhar, A. K. Nayak, Y. Sun, M. Schmidt, M. Nicklas, I. Leermakers, U. Zeitler, Y. Skourski, J. Wosnitzer, Z. Liu *et al.*, Extremely large magnetoresistance and ultrahigh mobility in the topological Weyl semimetal candidate NbP, *Nat. Phys.* **11**, 649 (2015).
- [33] I. A. Smirnov and V. S. Oskotski, Thermal conductivity of rare earth compounds, in *Handbook on the Physics and Chemistry of Rare Earths*, Vol. 16, edited by K. A. Gschneidner, Jr., J.-C. G. Bünzli, and V. K. Pecharsky (Elsevier, Amsterdam, 1993), pp. 107–224.
- [34] D. Flavian, J. Nagl, S. Hayashida, M. Yan, O. Zaharko, T. Fennell, D. Khalyavin, Z. Yan, S. Gvasaliya, and A. Zheludev, Magnetic phase diagram of the breathing-kagome antiferromagnet Nd<sub>3</sub>BWO<sub>9</sub>, *Phys. Rev. B* **107**, 174406 (2023).
- [35] D. Vu, W. Zhang, C. Şahin, M. E. Flatté, N. Trivedi, and J. P. Heremans, Thermal chiral anomaly in the magnetic-field-induced ideal Weyl phase of Bi<sub>1-x</sub>Sb<sub>x</sub>, *Nat. Mater.* **20**, 1525 (2021).
- [36] P. K. Tanwar, M. Ahmad, M. S. Alam, X. Yao, F. Tafti, and M. Matusiak, Gravitational anomaly in the ferrimagnetic topological Weyl semimetal NdAlSi, *Phys. Rev. B* **108**, L161106 (2023).
- [37] X. C. Huang, L. X. Zhao, Y. J. Long, P. P. Wang, D. Chen, Z. H. Yang, H. Liang, M. Q. Xue, H. M. Weng, Z. Fang *et al.*, Observation of the chiral-anomaly-induced negative magnetoresistance in 3D Weyl semimetal TaAs, *Phys. Rev. X* **5**, 031023 (2015).
- [38] C. Kittel, Interaction of spin waves and ultrasonic waves in ferromagnetic crystals, *Phys. Rev.* **110**, 836 (1958).
- [39] H. Jin, O. D. Restrepo, N. Antolin, S. R. Boona, W. Windl, R. C. Myers, and J. P. Heremans, Phonon-induced diamagnetic force and its effect on the lattice thermal conductivity, *Nat. Mater.* **14**, 601 (2015).
- [40] X. F. Sun, I. Tsukada, T. Suzuki, S. Komiya, and Y. Ando, Large magnetothermal effect and spin-phonon coupling in a parent insulating cuprate Pr<sub>1.3</sub>La<sub>0.7</sub>CuO<sub>4</sub>, *Phys. Rev. B* **72**, 104501 (2005).
- [41] D. D. Vu, R. A. Nelson, B. L. Wooten, J. Barker, J. E. Goldberger, and J. P. Heremans, Magnon gap mediated lattice thermal conductivity in MnBi<sub>2</sub>Te<sub>4</sub>, *Phys. Rev. B* **108**, 144402 (2023).
- [42] S. Guang, N. Li, R. L. Luo, Q. Huang, Y. Wang, X. Yue, K. Xia, Q. Li, X. Zhao, G. Chen *et al.*, Thermal transport of fractionalized antiferromagnetic and field induced states in the Kitaev material Na<sub>2</sub>Co<sub>2</sub>TeO<sub>6</sub>, *Phys. Rev. B* **107**, 184423 (2023).
- [43] C. Schindler, S. Galeski, W. Schnelle, R. Wawrzyńczak, W. Abdel-Haq, S. N. Guin, J. Kroder, N. Kumar, C. Fu, H. Borrmann *et al.*, Anisotropic electrical and thermal magnetotransport in the magnetic semimetal GdPtBi, *Phys. Rev. B* **101**, 125119 (2020).
- [44] D. Walton, J. E. Rives, and Q. Khalid, Thermal transport by coupled magnons and phonons in yttrium iron garnet at low temperatures, *Phys. Rev. B* **8**, 1210 (1973).
- [45] R. Jin, Y. Onose, Y. Tokura, D. Mandrus, P. Dai, and B. C. Sales, In-plane thermal conductivity of Nd<sub>2</sub>CuO<sub>4</sub>: Evidence for magnon heat transport, *Phys. Rev. Lett.* **91**, 146601 (2003).
- [46] A. Kobińska, M. Sternik, and A. Ptak, Dynamical properties of the magnetic topological insulator TBi<sub>2</sub>Te<sub>4</sub> ( $T = \text{Mn, Fe}$ ): Phonons dispersion, Raman active modes, and chiral phonons study, *Phys. Rev. B* **105**, 214304 (2022).
- [47] L. Zhang and Q. Niu, Chiral phonons at high-symmetry points in monolayer hexagonal lattices, *Phys. Rev. Lett.* **115**, 115502 (2015).
- [48] J. Skórka, K. J. Kapcia, P. T. Jochym, and A. Ptak, Chiral phonons in binary compounds ABi ( $A = \text{K, Rb, Cs}$ ) with  $P2_1/c$  structure, *Mater. Today Commun.* **35**, 105888 (2023).
- [49] D. M. Juraschek and N. A. Spaldin, Orbital magnetic moments of phonons, *Phys. Rev. Mater.* **3**, 064405 (2019).
- [50] G. Schaack, Observation of circularly polarized phonon states in an external magnetic field, *J. Phys. C: Solid State Phys.* **9**, L297 (1976).
- [51] D. M. Juraschek, T. Neuman, and P. Narang, Giant effective magnetic fields from optically driven chiral phonons in 4f paramagnets, *Phys. Rev. Res.* **4**, 013129 (2022).
- [52] S. Park and B.-J. Yang, Topological magnetoelastic excitations in noncollinear antiferromagnets, *Phys. Rev. B* **99**, 174435 (2019).
- [53] S. Pailhès, X. Fabrèges, L. P. Régnault, L. Pinsard-Godart, I. Mirebeau, F. Moussa, M. Hennion, and S. Petit, Hybrid Goldstone modes in multiferroic YMnO<sub>3</sub> studied by polarized inelastic neutron scattering, *Phys. Rev. B* **79**, 134409 (2009).
- [54] L. J. Cornelissen, K. Oyanagi, T. Kikkawa, Z. Qiu, T. Kuschel, G. E. W. Bauer, B. J. van Wees, and E. Saitoh, Nonlocal magnon-polaron transport in yttrium iron garnet, *Phys. Rev. B* **96**, 104441 (2017).
- [55] K. Uchida, H. Adachi, T. An, T. Ota, M. Toda, B. Hillebrands, S. Maekawa, and E. Saitoh, Long-range spin Seebeck effect and acoustic spin pumping, *Nat. Mater.* **10**, 737 (2011).
- [56] N. Zhang, D. Tu, D. Li, K. Tang, L. Nie, H. Li, T. Qi, T. Wu, J. Zhou, Z. Xiang, and X. Chen, Abnormally enhanced Hall

- Lorenz number in the magnetic Weyl semimetal NdAlSi, *Nat. Commun.* **15**, 10255 (2024).
- [57] C. C. Gu, Z. Y. Zhao, X. L. Chen, M. Lee, E. S. Choi, Y. Y. Han, L. S. Ling, L. Pi, Y. H. Zhang, G. Chen *et al.*, Field-driven quantum criticality in the spinel magnet  $\text{ZnCr}_2\text{Se}_4$ , *Phys. Rev. Lett.* **120**, 147204 (2018).
- [58] N. C. Drucker, T. Nguyen, F. Han, P. Siriviboon, X. Luo, N. Andrejevic, Z. Zhu, G. Bednik, Q. T. Nguyen, Z. Chen *et al.*, Topology stabilized fluctuations in a magnetic nodal semimetal, *Nat. Commun.* **14**, 5182 (2023).
- [59] P. E. Blochl, Projector augmented-wave method, *Phys. Rev. B* **50**, 17953 (1994).
- [60] G. Kresse and J. Hafner, *Ab initio* molecular-dynamics simulation of the liquid-metal–amorphous-semiconductor transition in germanium, *Phys. Rev. B* **49**, 14251 (1994).
- [61] G. Kresse and J. Furthmüller, Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set, *Phys. Rev. B* **54**, 11169 (1996).
- [62] G. Kresse and D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method, *Phys. Rev. B* **59**, 1758 (1999).
- [63] J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized gradient approximation made simple, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [64] S. L. Dudarev, G. A. Botton, S. Y. Savrasov, C. J. Humphreys, and A. P. Sutton, Electron-energy-loss spectra and the structural stability of nickel oxide: An LSDA+U study, *Phys. Rev. B* **57**, 1505 (1998).
- [65] H. J. Monkhorst and J. D. Pack, Special points for Brillouin-zone integrations, *Phys. Rev. B* **13**, 5188 (1976).
- [66] K. Parlinski, Z. Q. Li, and Y. Kawazoe, First-principles determination of the soft mode in cubic  $\text{ZrO}_2$ , *Phys. Rev. Lett.* **78**, 4063 (1997).
- [67] A. Togo and I. Tanaka, First principles phonon calculations in materials science, *Scr. Mater.* **108**, 1 (2015).
- [68] T. Tadano, Y. Gohda, and S. Tsuneyuki, Anharmonic force constants extracted from first-principles molecular dynamics: Applications to heat transfer simulations, *J. Phys.: Condens. Matter* **26**, 225402 (2014).
- [69] T. Tadano and S. Tsuneyuki, First-principles lattice dynamics method for strongly anharmonic crystals, *J. Phys. Soc. Jpn.* **87**, 041015 (2018).