Magneoelastic coupling enabled tunability of magnon spin current generation in 2D antiferromagnets

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We theoretically investigate the magnetoelastic coupling (MEC) and its effect on magnon transport in two-dimensional antiferromagnets with a honeycomb lattice. MEC coefficient along with magnetic exchange parameters and spring constants are computed for monolayers of transition-metal trichalcogenides with Néel order (MnPS3 and VPS3) and zigzag order (CrSiTe3, NiPS3 and NiPSe3) by ab initio calculations. Using these parameters, we predict that the spin-Nernst coefficient is significantly enhanced due to magnetoelastic coupling. Our study shows that although Dzyaloshinskii-Moriya interaction can produce spin-Nernst effect in these materials, other mechanisms such as magnon-phonon hybridization and enhancement of the Berry curvature and thus the spin-Nernst coefficient. Our results pave the way towards gate tunable spin current generation in 2D magnets by SNE via electric field modulation of MEC and anisotropy.

Recently, there is a growing interest in antiferromagnets (AFMs) as promising material platforms in spintronics. Because of the intrinsic timescale at THz range and the absence of the stray field, antiferromagnetic materials specially two dimensional (2D) AFMs [1–3] due to their reduced dimension are excellent candidates for high-speed and compact devices. Several interesting phenomena have been studied on AFMs such as the spin Hall effect [4–7], thermal Hall effect [8–10] and spin Nernst effect (SNE) [11–15]. In case of SNE, an experimental demonstration in MnPS3 was first attributed to the presence of the Dzyaloshinskii-Moriya interaction (DMI) [16]. However, the DMI in MnPS3 was later found to be too small to be responsible for this effect [17]. In one hand, it is well known that the Berry curvature plays a crucial role on the transport of collective excitations in various systems [18–20]. On the other hand, a magnetoelastic wave (hybridized excitation of magnons and phonons [21]), can carry large Berry curvature in the anticrossing regions between the magnon and phonon bands. These excitations which originate from the magnetoelastic coupling (MEC), can exhibit nontrivial topology even in the systems with trivial topology [22–24]. Therefore, the MEC can be an important mechanism for inducing large SNE in AFMs [46].

MEC has been considered in ferromagnetic materials with a square [25] or honeycomb lattice [26] and in AFMs with a square lattice [27] in both magnon and phonon transport properties. Though these studies provide insight on the importance of the MEC in magnon transport, they do not deal with the realistic materials. In this work, we choose transition-metal trichalcogenides (TMTCs) with honeycomb magnetic lattices because several magnetic phases especially AFM orders have been observed in these materials. Moreover, TMTCs are layered compounds with weak interlayer van der Waals interactions and are therefore excellent candidates for 2D AFMs [28–34].

We introduce a four-state method for calculating the MEC coefficients based on first-principles calculations in the framework of the density functional theory (DFT). Force constants are calculated by finite difference [35] while the values for symmetric exchange interactions up to the third nearest neighbor as well as the second nearest neighbor DMI interactions are taken from Ref. 15. Using these parameters we obtain the SNE coefficient for Néel (MnPS3 and VPS3) and zigzag (CrSiTe3, NiPS3 and NiPSe3) ordered TMTCs. Our results show that including the MEC enhances the SNE coefficients by one or two orders of magnitude. Furthermore, our study shows that magnetic anisotropy plays a crucial role in the magnon-phonon hybridization and thus SNE. These findings suggest a way for tunability and control of SNE generated spin current via modulation of MEC and anisotropy with e.g. applying a gate voltage.

We perform DFT+U calculations as implemented in QUANTUM ESPRESSO [36] with the Rappe-Rabe-Kaxiras-Joannopoulos ultrasoft (RRKJUS) pseudopotentials, the Perdew-Burke-Ernzerhof (PBE) formalism of the generalized gradient approximation (GGA) [37] and a kinetic energy cutoff of 400 eV. The Hubbard potential parameters are assumed as 5, 3, 2.5, 4 and 6.45 eV for Mn, V, Cr and Ni, respectively [32]. A tight convergence threshold of $10^{-7}$ eV is assumed for the total

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energy. A vacuum region larger than 20 Å is used for each slab. Structural optimization are done while fixing the in-plane lattice constants to those reported in Refs. 31 and 32. The magnetic ions A (Mn, V, Cr, Ni) make a honeycomb lattice with B$_2$X$_6$ ligands on the center of a hexagon made by A atoms. (c) Schematic representation of the four states used to calculate the MEC coefficient. The big arrows represent the spin of two neighboring magnetic atoms while the smaller one indicates the out-of-plane displacement of one of them.

In the investigated TMTCs with honeycomb magnetic lattice the spins possess Néel or zigzag ordering with out of plane spin orientation. The magnetic atoms can move out of plane and thus MEC comes into the play. Total Hamiltonian reads $H = H_m + H_{ph} + H_{mp}$. We write the magnetic Hamiltonian as

$$H_m = J_1 \sum_{(ij)} S_i \cdot S_j + J_2 \sum_{(ij)} S_i \cdot S_j + J_3 \sum_{(ijk)} S_i \cdot S_j + D_2 \sum_{(ij)} \xi_{ij} \hat{z} \cdot (r_{ik} \times r_{kj}),$$

where $J_1$, $J_2$ and $J_3$ are the Heisenberg exchange interaction parameters between the first, second, and third nearest neighbor spins, respectively. $D_2$ is the DMi parameter in the $z$ direction, $S_i$ is the total spin at site $i$, and $\xi_{ij}$ = sgn $\sum_{(i,k),(k,j)} \hat{z} \cdot (r_{ik} \times r_{kj})$, where $r_{ij} = r_j - r_i$ with $r_i$ denoting the position of site $i$. The last two terms in Eq. (1) correspond to the easy-axis anisotropy and Zeeman coupling to external magnetic field, respectively. We apply the Holstein-Primakoff transformation [38] for spin $S_i = S^x_i \hat{x}_i + S^y_i \hat{y}_i + S^z_i \hat{z}_i$, where $S^x_i = \sqrt{2S}(a_i + a_i^\dagger)/2$, $S^y_i = \sqrt{2S}(a_i - a_i^\dagger)/2i$ and $S^z_i = S - a_i a_i^\dagger$. The local spin coordinates for upward spins coincide the global coordinates while for downward spins $\hat{x}_i = -\hat{y}$ and $\hat{z}_i = -\hat{z}$.

For each magnetic atom of mass $M$, only its out-of-plane displacements, $u_i$, is relevant to the MEC [27]. The corresponding phonon Hamiltonian is therefore given by

$$H_{ph} = \frac{1}{2M} \sum_i p_i^2 + \frac{K_i^2}{2} \sum_{(ij)} u_{ij}^2$$

where $p_i$ denotes the linear momentum of atom $i$, $K_i^2$ is the nearest neighbor transverse spring constant and $u_{ij} = u_i - u_j$ is correspondingly the distance between the out-of-plane positions of two nearest neighbors. Finally, the magnon-phonon coupling part of the Hamiltonian arising from MEC in an AFM honeycomb lattice is described to the linear order by [25, 26, 39]

$$H_{mp} = \kappa \sum_{(ij)} \lambda_i (S_i \cdot \hat{r}_{ij}) u_{ij}$$

where $\kappa$ is the magnetoelectric constant and $\hat{r}_{ij} = r_{ij}/r_{ij}$. Note that Eq. (3) is valid only if $\lambda_i = S^z_i/S \approx \pm 1$.

The numerical values of coefficients in Eqs. (1), (2) and (3) are listed in Table I. The values of $J_1$, $J_2$, $J_3$ and $D_2$ are those previously determined from first principles calculations by a four-state method Ref. 15. $K_i^2$ is calculated by finite difference method from DFT+U energies. For calculating $\kappa$, we adopt the following four-state method. In short, all the spins in the supercell are set parallel to the $z$-axis while the spin of atom at a given site $i$ is slightly tilted toward or away from a nearest neighbor atom at site $j$ which is displaced normal to the sheet plane either upward or downward by a tiny value, e.g. $u = 0.05 \text{ Å}$. The four possible configurations of a pair of atoms highlighted in Fig. 1(a) are:

- state I: $S_i = (0, +S_y, S_z)$ and $u_j = +u$
- state II: $S_i = (0, -S_y, S_z)$ and $u_j = +u$
- state III: $S_i = (0, +S_y, S_z)$ and $u_j = -u$
- state IV: $S_i = (0, -S_y, S_z)$ and $u_j = -u$

as illustrated schematically in Fig. 1(c). A value of $S_y = \pm 0.3S$ which leads to $\lambda_i = \pm 0.954$, fulfills the validity requirements for Eq. (3) as discussed before. It can be easily shown that the MEC coefficient reads

$$\kappa = \frac{1}{4S_yu} (E_{II} + E_{III} - E_I - E_{IV}),$$

where $E_I$, $E_{II}$, $E_{III}$ and $E_{IV}$ are the DFT+U energies of the four states defined in Eq. (4).

To obtain the band structure of the excitations the total bosonic BdG Hamiltonian in the Fourier space,

$$H = \frac{1}{2} \sum_k \phi^\dagger_k \mathcal{H}(k) \phi_k$$

is diagonalized using the Colpa’s method [15, 24, 44] (for
TABLE I. Magnetic ground state, lattice constant (Å), magnetic moment per TM atom, exchange (meV) and DMI parameters (meV Å), Néel temperature (K) from Monte Carlo simulations and experiment, anisotropy coefficient (meV), transverse spring constant (meV Å²) and MEC coefficient (meV Å) for the five investigated TMTCs. The two columns on the right are calculated in this work. The first eight columns are adopted from Ref. [15]. K (meV) is set to the available experimental values for bulk MnPS₃ [29] and NiPS₃ [40]. For NiPS₃ and VPS₃ no experimental K is available while the experimental values for bulk CrSiTe₃ [41] makes our 2D calculation numerically unstable (We note that the GS 2D CrSiTe₃ is zigzag [31] while it is ferromagnetic in bulk [41]). Therefore, for NiPS₃ we use the same K value as NiPS₃, and for VPS₃ and CrSiTe₃ we took the smallest values that lead to stable numerical solutions.

| Material     | GS     | a     | S/μ₅B | J₁ | J₂ | J₃ | D₂₂ | MC | Exp | K     | K_i  |
|--------------|--------|-------|-------|----|----|----|-----|----|-----|-------|------|
| MnPS₃        | Néel   | 5.88  | 4.56  | 0.527 | 0.024 | 0.150 | 0.39 | 150 | 78 [29] | -0.002 | 479.9 | 0.0292 |
| VPS₃         | Néel   | 5.85  | 2.82  | 7.387 | 0.068 | 0.223 | 7.23 | 530 | -   | -0.014 | 106.7 | 0.6858 |
| CrSiTe₃      | zigzag | 6.84  | 3.76  | -0.990 | 0.009 | 0.389 | 39.00 | 48  | 80 [42] | -0.23  | 118.9 | 0.9320 |
| NiPS₃        | zigzag | 5.82  | 1.58  | -1.039 | -0.163 | 3.882 | 4.54 | 105 | 150 [43] | -0.190 | 243.6 | 0.2949 |
| NiPSe₃       | zigzag | 6.14  | 1.56  | -1.131 | -0.069 | 3.975 | 43.90 | 110 | -   | -0.190 | 173.8 | 1.9729 |

FIG. 2. Magnetic unit cell for (a) the Néel phase and (b) zigzag phase. Symmetry points for (c) the Néel phase and (d) zigzag phase. The band structure and density of states (DOS) of (e) MnPS₃, (f) VPS₃, (g) CrSiTe₃, (h) NiPS₃ and (i) NiPSe₃. The spin character |⟨S^z⟩| of the modes is indicated with colors.

The generalized Berry curvature of the nth band is given by [47]

\[
(\Omega_n^\theta(k))_{xy} = \sum_{m \neq n} 2i \langle n|\theta_x|m\rangle \langle m|\theta_y|n\rangle (\hat{\varphi}_{mn}(\hat{\varphi})_{nm}) \left(\langle\hat{\varphi}E\rangle_{nn} - (\hat{\varphi}E)_{nm}\right)^2
\]

where the index k is dropped for simplicity (the conventional Berry curvature is presented in the SM [45]). The SNE coefficient is defined as \(\alpha_{xy}\) \(\equiv j_{SNE}/(\hat{z} \times \hat{T})\) [11], where \(\hat{T}\) is an in-plane temperature gradient and the magnon spin current, \(j_{SNE}\) is calculated based on the linear response theory [46, 47] as

\[
\alpha_{xy} = 2k_B \sum_{n=1}^N \int dk (\Omega_n^\theta(k))_{xy} c_1 \left(\frac{E_{nn}}{k_B T}\right)
\]

where \(c_1(x) = [1 + \rho(x)] \log[1 + \rho(x)] - \rho(x) \log \rho(x)\) and \(\rho(x) = 1/(e^x - 1)\). Note that only the particle bands (the first N bands) contribute to the summation.

In an experimental report a bulk crystal of MnPS₃ was used whose edges are cut at an inclination angle \(\eta = 45^\circ\) and Pt stripes were used as electrodes [16]. To get results...
comparable with such SNE measurement in TMTCs, we adopt the SNE signal introduced in Ref. 15

$$S_{\text{SNE}} = \frac{V_{\text{SNE}}}{\Delta T} = \frac{e}{\hbar d} \rho_{\text{SH}} \sigma_{xy}^s \cos \eta. \quad (10)$$

where $V_{\text{SNE}}$ is voltage due to inverse spin Hall effect, $\Delta T$ is the temperature difference across the length of Pt stripes, $d$ is the inter-layer distance in the TMTC, and $\rho = 10^{-6} \, \Omega/m$ and $\theta_{\text{SH}} = 0.15$ are the electrical resistivity and the spin Hall angle of Pt, respectively.

All the parameters for constructing the Hamiltonian, including the calculated MEC coefficients $\kappa$ and transverse spring constant $K_{\perp}$, are reported in Table I. The resulting band structure along the high symmetry directions shown in Figs. 2(c) and (d) as well as the density of states (DOS) of the quasiparticle bands are presented in Figs. 2(e-i) and (g-i) for the Néel and zigzag ordered materials, respectively. From the absolute value of the $z$-component of spin, $|\langle S^z \rangle|$ [45], encoded by the color bar in the band structure plots, one clearly identifies two degenerate magnon bands (red) and two phonon bands (blue) in the Néel phase. On the other hand, four magnon bands (two doubly-degenerate bands) and four phonon bands are identified for the zigzag phase.

As can be seen in Fig. 2, MEC leads to hybridization of magnon and phonon bands which manifests itself as the anticrossing regions (some of anticrossing regions are shown in Fig. S6). Therefore, the generalized Berry curvature becomes very large in these anticrossing regions for both Néel and zigzag ordered materials, as illustrated in Figs. S3 and S4 of the SM [45]. Consequently, the SNE coefficient is largely increased as seen in Fig. 3. By including the MEC in the calculations, the maximum SNE coefficient within the shown temperature range is enhanced by a factor of $\sim23$, 12, 13, 620 and 99 for MnPS$_3$, VPS$_3$, CrSiTe$_3$, NiPS$_3$ and NiPSe$_3$, respectively.

A log-log plot of the absolute value of SNE coefficient, $|\sigma_{xy}^s|$, as a function of the anisotropy $K$ at $T = 50 \, K$ is also depicted in the insets of Fig. 3 (Note that there is a sign change at $K = -0.004$ meV for MnPS$_3$). It is clearly seen that the SNE coefficient is fairly sensitive to changes in the anisotropy. This is due to the effect of anisotropy in displacing bands and thus anticrossing regions which in turn changes the generalized Berry curvature and SNE.

There are also other factors that affect SNE coefficient. For MnPS$_3$ and VPS$_3$, there are anticrossing region at higher energies (around 8 meV) leading to different behavior at higher temperatures (around 90 K). The situation is more complicated for zigzag ordered materials due to magnon-phonon hybridization in several regions. Specially, for CrSiTe$_3$ we can see large generalized Berry curvature almost everywhere in the Brillouin zone (Fig. S4) which leads to very large SNE coefficient compared to other materials. For NiPS$_3$ and NiPSe$_3$, we see anticrossing regions around the M and $\Gamma$ points (See Figs. 2(h) and (i)). However, relatively small generalized Berry curvature is induced near the $\Gamma$ point (see Fig. S4). We thus consider only the anticrossing regions around the M point. For both materials the hybridization is stronger at the anticrossing with lower energies. However, since the MEC coefficient $\kappa$ of NiPSe$_3$ is very large, the magnon bands which carry $+1$ and $-1$ spins and the phonon bands strongly mix at this region (around the M point). This results in magnon bands with almost no spin, i.e. the spin sectors with opposite spins cancel each other (shown in Figs. S5 (n) and (o) where the lower bands around the M point have considerable magnon contents but almost no spin), so they have less contribution to the SNE coefficient. On the other hand, $\kappa$ of NiPS$_3$ is much smaller, thus there are still bands that can carry spin at the anticrossings around the M point with lower energies. So the lower bands mainly contribute to the SNE coefficient (see Fig. S4), and their contribution is negative leading to negative SNE coefficient. In contrast, the anticrossings around the M point with higher energies (higher bands at it can be seen in Fig. S4) contributes mainly to the SNE coefficient of NiPS$_3$ and their contribution is positive.

We also note that the individual contribution of each band to SNE coefficient can be orders of magnitude larger than the final SNE (see Fig. S7). However, the sum of positive bands is almost equal to negative bands but opposite in sign (see the inset of Fig. S7). So there is very small difference between the absolute values of positive and negative bands which leads to very small SNE coefficient compared to the contribution of each band yet much larger than SNE coefficient in the absence of MEC. In contrast, when $\kappa = 0$ the contribution of each band is comparable with final SNE coefficient.

In summary, this study reveals that MEC induces large generalized Berry curvatures in anticrossing regions which in turn translates into large SNE in TMTC materials. We also found that the SNE is sensitive to anisotropy and paves the way for designing tunable spintronic devices. Among the TMTC materials studied in this work, NiPSe$_3$ has the largest MEC, but the largest SNE is observed in CrSiTe$_3$. Despite the focus of previous studies, presence of DMI cannot explain large SNE observed in MnPS$_3$ [16]. Other magnon-phonon coupling mechanisms should be also considered in the future works to better understand the topological properties of TMTC antiferromagnets.

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FIG. 3. The SNE coefficient (blue dashed lines) and SNE signal (red dashed lines) versus temperature, top for Néel phase and bottom for zigzag phase. The experimental and Monte Carlo Néel temperatures are also marked with vertical black dashed lines. Insets: The SNE coefficient in terms of easy-axis anisotropy $K$ plotted in logarithmic scale.

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