Atomistic Simulation of Phonon and Magnon Thermal Transport across the Ferro-Paramagnetic Transition

Yanguang Zhou, Julien Tranchida, Yijun Ge, Jayathi Murthy, and Timothy S. Fisher

1Mechanical and Aerospace Engineering Department, University of California Los Angeles, Los Angeles, CA 90095, USA
2Multiscale Science Department, Sandia National Laboratories, P.O. Box 5800, MS 1322, Albuquerque, NM 87185, USA

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A temperature-dependent approach involving Green-Kubo equilibrium spiral and atomic dynamics (GK-ESAD) is reported to assess phonon and magnon thermal transport processes accounting for phonon-magnon interactions. Using body-center cubic (BCC) iron as a case study, GK-ESAD successfully reproduces its characteristic temperature-dependent spiral and lattice thermal conductivities. The non-electronic thermal conductivity, i.e., the summation of phonon and magnon thermal conductivities, calculated using GK-ESAD for BCC Fe agrees well with experimental measurements. Spectral energy analysis shows that high-frequency phonon-magnon scattering rates are one order magnitude larger than those at low frequencies due to energy scattering conserving rules and high density of states. Higher temperatures further accentuate this phenomenon. This new framework fills existing gaps in simulating thermal transport across the ferro- to para-magnetic transition. Future application of this methodology to phonon- and magnon-dominant insulators and semiconductors will enhance understanding of emerging thermoelectric, spin caloritronic and superconducting materials.

A better understanding of heat transfer considering interactions among different temperature-induced excitations in crystals, e.g., phonons, electrons and spins, is of great importance in many disciplines, including thermoelectric [1–3], spin caloritronic [4] and superconducting materials. Unlike phonons and electrons, whose thermal transport properties have been well studied, the heat transport behavior of magnons - collective excitations of magnetic spins - is poorly understood at the fundamental level. Little is known about the influence of phonon-magnon and magnon-magnon scattering on heat transfer. For example, the experimental lattice thermal conductivities of magnetic materials such as body-centered cubic (BCC) iron [9–11], face-centered cubic (FCC) nickel [8], YMnO₃, LuMnO₃ and ScMnO [9], as well as CrN [10–11], show significantly different temperature dependences near the Curie temperature (Tc), compared to the typical 1/T relation at high temperatures when only phonons are considered [12–14]. The magnetic configuration changes from a ferromagnetic state at low temperature in which spins are aligned to a paramagnetic state above the Curie temperature in which the spin configuration is fully disordered [15].

To model the thermal transport properties of magnetic materials, temperature-dependent lattice and magnetic excitations must be taken into consideration when calculating the inputs, e.g., heat current or force constants, for thermal conductivity. To date, theoretical studies have sought to develop explanations for mutual interactions between phonons and magnons [15–19]. However, most such studies provide only a partial treatment based on thermodynamic properties [15–19], average phonon-magnon relaxation times [16], and phonon-magnon temperature gradients [18]. A robust framework to compute thermal transport properties such as thermal conductivity and modal scattering rates in magnetic materials is still lacking.

In this letter, a temperature-dependent method - Green-Kubo equilibrium spiral and atomic dynamics (GK-ESAD) - based on linear response theory [21] and spin-lattice dynamics (SLD) [22] is reported to calculate the thermal transport properties of phonons and magnons in magnetic materials. In GK-ESAD, phonon-phonon scattering (PPS), phonon-magnon scattering (PMS) and magnon-magnon scattering (MMS) are inherently included. As a proof of concept, our study focuses on a model system consisting of a simple transition-metal ferromagnet, BCC iron, with a Curie temperature of 1043 K. Using this methodology, we successfully reproduce the characteristic temperature-dependent non-electronic thermal conductivity observed in experiments for magnetic materials [16–19, 23]. Modal phonon-phonon, magnon-magnon and phonon-magnon scattering rates are then quantified using spectral energy density (SED) analysis. The agreement between theoretical predictions and experimental measurements establishes the reliability of the methodology. Simulation details are available in the Supporting Materials [24].

The energy E of magnetic crystals must account for terms coupling the magnetic spins (E_{spin}) to the lattice (E_{kinetic} and E_{potential}) through the following expression [22]:

$$E = E_{kinetic} + E_{potential} + E_{spin}$$

$$= \sum_{i=1}^{N} \frac{|\vec{p}_i|^2}{2m_i} + \sum_{i,j=1}^{N} V(\vec{r}_{ij}) - \sum_{i,j}^{N} J(|\vec{r}_{ij}|) \vec{s}_i \cdot \vec{s}_j $$

(1)

in which \(\vec{r}, \vec{p}\) and \(\vec{s}\) are the position, momentum and spin vectors of the atoms, respectively. The negative sign on the last term indicates that the ground state energy of the system considering spin becomes lower. \(J(|\vec{r}_{ij}|)\) is...
the magnetic coupling exchange constant, which originates from two main contributions: (i) direct ferromagnetic exchange between the orbitals localized on centers of ions \(i\) and \(j\), and (ii) spin and charge polarizations effects brought by nonmagnetic orbitals. Phonons and magnons are coupled in Eq. (1) via the atomistic positions, i.e., \(\vec{r}_{ij}\). The heat flux due to lattice vibrations takes the form [23]

\[
Q_{\text{lattice}}^{\vee} = \frac{1}{V} \sum_i \frac{d(E_i^{\text{kinetic}} + E_i^{\text{potential}})}{dt} \vec{v}_i
\]

\[
= \frac{1}{V} \left\{ \sum_i e_i \cdot \vec{v}_i + \frac{1}{2} \sum_{i,j=1; j \neq i} \left( \vec{F}_{ij} \cdot \vec{v}_i \right) \cdot \vec{r}_{ij} \right\} \tag{2}
\]

and the heat flux associated with spin is expressed as [24]

\[
Q_{\text{spin}}^{\vee} = \frac{1}{2A} \sum_i \frac{dE_i^{\text{spin}}}{dt}
\]

\[
\approx \frac{1}{2A} \sum_{i \in \text{Right}, j \in \text{Left}} \sum_j \left( J_{ij}(\vec{r}_{ij}) \left( \frac{d\vec{s}_i}{dt} + \vec{v}_j \frac{d\vec{s}_j}{dt} \right) \right)
\]

\[
= -\frac{1}{k} \sum_{i \in \text{L}, \text{R}} \sum_j \left( J(\vec{r}_{ij}) \left( \frac{\partial E_{\text{spin}}}{\partial \vec{s}_j} \right) \times \vec{s}_j \right) \cdot \vec{s}_i \tag{3}
\]

where \(e_i\) and \(\vec{v}_i\) are the energy and the velocity of atom \(i\), respectively, \(\vec{F}_{ij}\) represents the force between two atoms, and \(V\) and \(A\) are the volume and the cross section area of the system, respectively. Based on linear response theory [21] and Eq. (2)-(3), the thermal conductivity of a magnetic system can be divided into contributions from lattice vibrations, \(\kappa_{\text{phonon}}\), spin-related fluctuations, \(\kappa_{\text{magnon}}\), and a term resulting from lattice-spin interactions, \(\kappa_{\text{cross}}\):

\[
\kappa = \kappa_{\text{phonon}} + \kappa_{\text{magnon}} + \kappa_{\text{cross}}
\]

\[
= \frac{V}{k_b T^2} \int \left[ \left( \langle Q_{\text{lattice}}^{\vee}(t) \cdot Q_{\text{lattice}}^{\vee}(0) \rangle \right)_{\text{phonon}} + \left( \langle Q_{\text{spin}}^{\vee}(t) \cdot Q_{\text{spin}}^{\vee}(0) \rangle + 2 \langle Q_{\text{spin}}^{\vee}(t) \cdot Q_{\text{lattice}}^{\vee}(0) \rangle \right)_{\text{cross}} \right] dt \tag{4}
\]

where \(k_b\) is the Boltzmann constant, and \(T\) is the temperature of the system. We note that \(\kappa_{\text{cross}}\) is not the result of phonon-magnon scattering, but of the cross-correlation between the phonon and magnon heat fluxes. Physically, the cross term represented the interaction between the heat carried by the phonons and the heat carried by the magnons that can alter pure phonon and spin heat flow. The effect of magnon scattering on phonon transport is elucidated by calculating the phonon thermal conductivity using \((E = E_{\text{kinetic}} + E_{\text{potential}} + E_{\text{spin}})\) and \((E = E_{\text{kinetic}} + E_{\text{potential}})\) and comparing the two values. Similarly, the influence of phonon scattering on magnon thermal conductivity is assessed by computing the magnon thermal conductivity using \((E = E_{\text{kinetic}} + E_{\text{potential}} + E_{\text{spin}})\) and \((E = E_{\text{spin}})\) and comparing the two values.

From Eqs. (2) and (3), the net heat flux of lattice vibrations \(Q_{\text{lattice}}^{\vee}\) and spin fluctuations \(Q_{\text{spin}}^{\vee}\) in EMD simulations should be zero, which is validated by our numerical results (Figure 1a and 1b). Furthermore, following linear response theory, the thermal conductivity of the two heat carriers should converge with the increasing correlation time [Eq. (4)], and this is also reflected in our simulations (Figure 1c).

To evaluate thermal conductivity behavior at different temperatures, the order of the spin configuration in our system is calculated via [30]

\[
P_{\text{order}} = \sqrt{\sum_{\alpha=x,y,z} \left( \sum_i s_{i,\alpha}^{T} \right)^2 / \sum_{\alpha=x,y,z} \left( \sum_i s_{i,\alpha}^{T=0} \right)^2}
\]

where \(P_{\text{order}} = 1\) in the ferromagnetic limit and \(P_{\text{order}} = 0\) in the paramagnetic limit. Small values of \(P_{\text{order}}\) indicate that spins in the system are predominantly disordered, which leads to broken periodicity.

By considering the contributions of both phonons and magnons [24], the predicted total thermal conductivity is in broad agreement with experimental measurements [6,7] over the temperature range from 300 K to 1200 K (Figure 2a) (the electrical thermal conductivity was subtracted from the experimental measurements). We note that the two experimental results [6,7] in Figure 2a are themselves quite different from each other, and the disagreement between them is larger than that caused by phonon-magnon scattering in the simulations. Thus, they cannot definitively establish the accuracy of our phonon-magnon scattering models. A number of reasons may account for these differences: (i) loss of heat from the specimen due to conduction through leads; (ii) impurities in the sample, which in Ref. [6] may be as high as 1%. An important feature in Figure 2a is the sharp fall in thermal conductivity reported in the experimental data of Ref.
magnon scattering is weak in a system, phonon or magnon thermal conductivity will be affected strongly by phonon-magnon scattering. We explore this effect by increasing $J$ by a factor of ten above its original value, i.e., with the system in a ferromagnetic state across the entire temperature range considered here (Figure 2b). The non-electronic thermal conductivity is found to become much higher than that at the original $J$ value and is dominated by magnons [24] (see Figure 8 in Supplemental Information). The thermal conductivity is then strongly affected by phonon-magnon scattering, is nearly temperature-independent, and phonon-magnon scattering decreases thermal conductivity by a factor of approx. 3 at room temperature.

To further understand the temperature behavior of thermal conductivity, mode-level phonon and magnon scattering rates have been calculated at three temperatures, 300 K, 700 K and 1100 K, by SED analysis [24]:

$$|\Phi|^2 = \frac{I_p}{(\omega - \omega_p)/\Delta}^2 + 1$$

where $I_p$ and $\omega_p$ are the peak magnitude and frequency at the peak center, respectively. $\Delta$ is the linewidth, which is half of the scattering rate $\Gamma$. $\Phi$ is the spectral energy, which takes the following form for phonons [37, 38]:

$$\Phi(q, \nu) \sim \frac{1}{\sqrt{2\pi \hbar \nu_0}} \int_0^{t_0} \sum_{jl} m_j \exp[i\vec{q} \cdot \vec{r}(jl) - i\omega t] \cdot \epsilon^0(jl, t) dt$$

and, for magnons, can be written as [41]:

$$\Phi(k, \mu) \sim \frac{\hbar}{\sqrt{2\pi \hbar \nu_0}} \int_0^{t_0} \sum_{jl} \exp[i\vec{k} \cdot \vec{r}(jl) - i\omega t] \cdot \epsilon^0(jl, t) dt$$

where $\epsilon^0$ is the mode eigenvector of a phonon or magnon, and $\nu_0$ is the integration limit. Using Matthiessen’s rule, phonon-magnon ($\Gamma_{\text{phonon-magnon}}$) and magnon-phonon ($\Gamma_{\text{magnon-phonon}}$) scattering rates can be calculated via:

$$\Gamma_{\text{phonon-magnon}} = \Gamma_{\text{magnon}} - \Gamma_{\text{no magnon}}$$

$$\Gamma_{\text{magnon-phonon}} = \Gamma_{\text{phonon}} - \Gamma_{\text{no phonon}}$$

where the superscripts magnon and no magnon indicate that the lattice vibrates with and without spins in the system, respectively [24], and vice versa for phonon and no phonon [24].

From the phonon-magnon scattering results (Figure 3), we observe a general tendency that high-frequency phonons ($\omega$ larger than 4.3 THz) are scattered by magnons more strongly than low-frequency phonons because the magnon energy is much larger than the phonon

FIG. 2: (a) The adjust total thermal conductivity for invariable and temperature dependent magnetic exchange coefficient $J$, and (b) adjust total thermal conductivity with strong magnetic exchange constant. The EMD results are averaged over 30 independent runs. The experimental results are the so-called “lattice thermal conductivities” in Ref. [7]. Here, the transition temperature for $J$ is 1000 K in case the results can fit the experimental measurements better.

near the Curie temperature (around 1200 K) due to the ferromagnetic-to-paramagnetic transition. Previously published atomic spin dynamics or spin lattice dynamics simulations have been known to smooth the ferromagnetic-to-paramagnetic phase transition near the Curie temperature [29, 31] (see $P_{\text{order}}$ with original $J$ in Figure 2a). One explanation is that the simulation of atomic spins is performed within a classical framework and ignores quantum effects [29, 34]. However, as previously demonstrated [24] and well established in Ref. [34], quantum effects can be ignored for phonon and magnon thermal transport properties in the temperature range considered here. Another explanation for the transition is that the value of the magnetic exchange parameter $J$ varies as a function of temperature [35, 39].

Our EMD simulations (black and blue symbols) in Figure 2a use a single, temperature-invariant value of $J$ and treat the spins as classical, and therefore the results do not exhibit the experimentally observed sharp fall in thermal conductivity. To explore this issue further, an additional set of computations was performed (open green symbols) wherein the value of $J$ varies with temperature. We assume that $J$ is constant when $T < T_c$, while $J$ is one tenth of the low temperature value when $T > T_c$. Thus, $P_{\text{order}}$ becomes zero when $T > T_c$ (Figure 2b), indicating that the spin configuration in the system is fully disordered (i.e., the paramagnetic limit). Consequently, the non-electronic thermal conductivity drops sharply around the Curie temperature due to the decrease in magnon thermal conductivity, consistent with the experimental observations [3, 7].

At the same time, phonon-magnon scattering does not exhibit a strong effect on thermal transport in BCC iron because the values of both the phonon and the magnon thermal conductivities are relatively small, i.e., phonon-phonon scattering and magnon-magnon scattering are the dominant scattering mechanisms in such materials. When phonon-phonon scattering or magnon-

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energy (Figure 3). For phonon-dominant magnetic materials in which the thermal conductivity is mainly due to phonons, magnons may scatter phonons [42, 43] through phonon emission or absorption, \( h \omega(\vec{k}', \mu') = h \omega(\vec{q}, \nu) + h \omega(\vec{k}, \mu) \). Referring to Figure 3c, and considering a magnon of energy \( h \omega_A \) scattered by a magnon of energy \( h \omega_B \), a high-frequency phonon would have a greater probability of involvement in a phonon-magnon scattering process than a low-frequency phonon. For instance, only two channels exist for the magnon \( h \omega_A \) to be scattered to the magnon \( h \omega_B \) when the phonon energy is \( h \omega = 12.41 \) meV (\( \omega = 3 \) THz), whereas the number of channels for the magnon \( h \omega_A \) to be scattered to the magnon \( h \omega_C \) is four when the phonon energy is \( h \omega = 37.6 \) meV (\( \omega = 9.1 \) THz, the highest phonon frequency). From the magnon dispersion curve, the frequency changes for the small (P1-P2) and large peaks (P2-P3) are 4.3 and 3.6 THz, respectively; therefore, phonons (magnons) above 4.3 (68) THz have a much greater chance to be involved in phonon-magnon scattering processes.

Another reason that high-frequency phonons are preferentially involved in phonon-magnon scattering processes is the high density of states of phonons in the high-frequency region (Figure 3c). First-principles calculations [15] and experimental measurements [44] also confirm that high-frequency phonons are more strongly scattered by magnons. For materials in which the magnon thermal conductivity is dominant, magnons are scattered by phonons [42, 43] via phonon absorption or emission processes \( h \omega(\vec{k}', \mu') \pm h \omega(\vec{q}, \nu) = h \omega(\vec{k}, \mu) \). The magnon-phonon scattering rate of high-frequency magnons is somewhat higher than that of low-frequency magnons (Figure 3b) because high-frequency magnons have a larger density of states (Figure 3c). The phenomena discussed above become more apparent at increased temperatures, which strengthen the scattering among the heat carriers.

To facilitate the analysis of thermal conductivity contributions, the thermal conductivity accumulation function has been computed with respect to the mean free path \( \Lambda \) using

\[
\kappa(\Lambda) = \sum_{\Lambda < \Lambda_0} c_v v_g \Lambda = \sum_{\Lambda < \Lambda_0} c_v v_g^2 \tau
\]  

(11)

where \( c_v, v_g \) [24] and \( \tau \) are the volumetric heat capacity, group velocity, and relaxation times of phonons and magnons, respectively. For phonons (Figure 4a), at \( T = 300 \) K, the accumulated thermal conductivities with and without spin are similar, indicating that magnons do not have a strong effect on phonon thermal conductivity near room temperature. This is due to the fact that long mean free path phonons are the main contributors to thermal conductivity, and these phonons do not easily scatter with magnons, as discussed above. However, at 700 K, the phonon mean free path falls to 0.3 - 4 nm, which is much smaller than that at 300 K due to strong phonon-phonon scattering (black triangle symbols in Figure 4a). Furthermore, high-frequency phonons with short mean free paths (0.4 - 0.8 nm) are more easily scattered by magnons. Consequently, the total lattice thermal conductivity of magnetic BCC iron becomes slightly smaller than that of non-magnetic BCC iron [24]. Finally, at 1100 K phonons are scattered strongly by both phonons and magnons because high
temperatures increase the vibration magnitude of lattice and spin excitations.

For magnons (Figure 4b) at room temperature, only the long-mean-free-path, or equivalently, low-frequency magnons are scattered by phonons because only these magnons transport significant energy, i.e., the heat capacity of high frequency magnons is very small [24]. When the system temperature increases to 700 K and then to 1100 K, the mean free path of magnons becomes much shorter than that at 300K, and the short mean free path (high frequency) magnons are scattered by phonons strongly.

We also note that the magnon group velocities are calculated here from the magnon dispersion without considering temperature effects, i.e., assuming a ferromagnetic system. Such an assumption may introduce inaccuracies in the magnon mean free path and modal thermal conductivity computations. At 300 K, the total magnon thermal conductivity calculated using BTE, i.e., using \( \kappa = \sum c_i v_i^2 \tau_i \) with the values of relaxation time computed using SED, is 10.1 W/mK. This value is lower than the BTE results of Wu et al. (15.2 W/mK) due to their overestimation of the magnon dispersion [11], whereas it is 7.8 W/mK computed by GK-ESAD. The closer correspondence between BTE and GK-ESAD at room temperature indicates that the system may be treated as ferromagnetic at 300 K. However, the total magnon thermal conductivities calculated by BTE (GK-ESAD) are 11.1 (1.9) and 56.9 (1.2) W/mK at 700 K and 1100 K, respectively. The large differences between SED-BTE and GK-ESAD indicate that the magnon group velocity is overestimated, and the calculation should consider spin disorder at high temperatures.

Before concluding our study, we briefly highlight two limitations that our methodology inherited from the SLD formalism. In our calculations, the exchange integral \( J_{ij} \) is assumed to remain constant, and its dependence on temperature is neglected. Recent studies have investigated this dependence and proposed methodologies to account for it [35, 36]. Encapsulating them within our framework could improve the accuracy of predictions. Furthermore, the simulation of classical spins (instead of quantum spins) is known to make the ferromagnetic to paramagnetic phase transition smoother than in the experimental observations. Implementing quantum baths and statistics has proven possible to reproduce more accurately the sharp transition occurring at \( T_c \) [29, 31]. However, as the GK-ESAD framework is based on equilibrium molecular dynamics, the associated simulations do not involve a connection to a random bath. Overall, an empirical parametrization of the exchange integral \( J_{ij} \) could account for both its temperature dependence and the sharp transition occurring at \( T_c \).

In conclusion, we have developed a temperature-dependent method, the Green-Kubo equilibrium spiral and atomic dynamics method, to calculate coupled phonon and magnon transport in magnetic materials. Reasonably good agreement is obtained between our simulation results and experimental measurements in computing dispersion curves and temperature dependent thermal conductivity, and these results suggests that the approach captures the overall heat transfer behavior of phonons and magnons in magnetic crystals. Analysis of scattering processes between phonons and magnons indicate that high-frequency phonon scattering rates due to phonon-magnon scattering are much larger than those at low frequencies because of energy-conserving rules for scattering and the high density of states. The application of this new methodology will yield deeper insights into the thermal transport properties of other phonon- or magnon-dominant materials.

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* Electronic address: jtranch@sandia.gov
† Electronic address: jmurthy@ucla.edu
‡ Electronic address: tsfisher@ucla.edu

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