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Model calculation of thermal conductivity in antiferromagnets

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ABSTRACT

A theoretical study is given of thermal conductivity in antiferromagnetic materials. The study has the advantage that the three-phonon interactions as well as the magnon phonon interactions have been represented by model operators that preserve the important properties of the exact collision operators. A new expression for thermal conductivity has been derived that involves the same terms obtained in our previous work in addition to two new terms. These two terms represent the conservation and quasi-conservation of wavevector that occur in the three-phonon Normal and Umklapp processes respectively. They gave appreciable contributions to the thermal conductivity and have led to an excellent quantitative agreement with the experimental measurements of the antiferromagnet $FeCl_2$.

1. Introduction

The thermal conduction in antiferromagnetic materials has been investigated by many authors. A variety of experimental works have been performed to measure the thermal conductivity of these materials over wide temperature ranges and in the presence and absence of magnetic fields. From the theoretical point of view considerable effort has been devoted to explore the role of the different heat carriers (phonons, magnons and electrons) and to interpret the strange anomalies that appear in the measurements. The thermal scattering mechanism arises mainly due to the interactions between the different types of carriers and between the carriers and the imperfections and impurities that may exist in antiferromagnetic materials.

The magnon–phonon interactions present one of the essential types of interactions that affect substantially the heat conduction in magnetic materials in general. For paramagnetic and ferromagnetic materials the situation is simpler than antiferromagnets. Elliott and Parkinson [1] explored the effect of magnon–phonon interactions on the thermal conductivity of Paramagnetic materials. Also Walton et al. [2] explained the magnetic field dependence of their thermal conductivity measurements of the ferromagnet yttrium iron garnet (YIG) at low temperatures (T=0.23–1 K) by taking into account both magnon and phonon contributions to the thermal current and considering a resonant one magnon one phonon interaction. Jensen and Hourmann [3] investigated further the role of the magnon–phonon interactions in the ferromagnet terbium. Also, considerable effort has been devoted to study the magnon–phonon interactions in ferromagnets by Wesselinowa [4,5] and Wesselinowa and Apostolov [6]. Their results were extended more recently to cover the cases of ferromagnetic thin films and nanoparticles [7,8]. Moreover, in last years great attention has been given to study the effect of magnon–phonon interactions on some important phenomena in ferromagnets [9–18].

In antiferromagnetic materials the situation is much more complicated. Slack and Newman [19] and Slack [20] considered the effect of magnon–phonon interactions using the relaxation time approximation. They introduced a simple expression for the relaxation time that depends on the magnetic order parameter. Mikhail [21] employed the expression obtained in Refs. [19,20] for the magnon–phonon interactions relaxation time. He succeeded to fit the measurements of Morelli et al. [22] on single crystal $La_2CuO_{4+\Delta}$ along the direction [001] and produced the sharp minimum anomaly that occurs at the Néel temperature. The magnon–phonon interactions were further investigated in La_2CuO_4 and related cuprates by Kochelaev [23]. Similar anomalies were detected in the measurements of thermal conductivity of other antiferromagnetic materials such as $FeCl_2$ [24,25] and $UNi_{0.5}Sb_2$ [26]. Mikhail et al. [27] re-stressed the importance of magnon–phonon interactions that were used to give a reasonable explanation of the anomalies displayed in the thermal conductivity

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measurements of Ref. [24].

Also, Gustafson and Walker [28] measured the thermal conductivity of the antiferromagnets $RbMnF_3$ and MnF_2 in the presence and absence of magnetic fields. They attributed the appreciable dependence of their measurements on the strength and direction of the field due to the coupling between spins and phonons. More recently Sales et al. [29] reported a strong dependence of the thermal conductivity and heat capacity of the antiferromagnet $K_2V_3O_8$ on the applied magnetic field. Very recent measurements have been performed [30] on the thermal conductivity, specific heat and thermal diffusivity to study the critical behavior of the antiferromagnetic transition in $KCoF_3$ and $KNiF_3$. We believe that the magnon–phonon interactions should play an appreciable role in investigating their measurements on thermal conductivity.

The importance of magnon–phonon interactions in antiferromagnets has been investigated recently in some fields other than thermal conduction. In this connection, Malard and Pires [31] have extended the results of Pires [18] on magnon–phonon interactions by using memory functions and perturbation expansions to be applied to the case of one dimensional antiferromagnets. Also, Khadikova et al. [32] have investigated the magnon–phonon interaction in the one dimensional Heisenberg spin-ladder antiferromagnet $La_5Ca_9Cu_{24}O_{41}$. For this purpose they performed the dynamical fluorescent micro-thermal imaging (FMI) experiment and modeled the dynamic heat transport experiment using a two temperature model approach. They took both the crystal and the polymer fluorescent heat imaging layer into account.

In view of the importance of magnon–phonon interactions in antiferromagnets several theoretical studies were performed to explore the effect of these interactions on the calculation of thermal conductivity by Gluck [33], Dixon [34], Dixon et al. [35] and Mikhail et al. [27]. Dixon [34] developed a model of two magnon–one phonon interactions in antiferromagnetic materials. He obtained two types of processes, the first is the conversion processes (C-processes) in which two magnons are created (or annihilated)and a phonon is destroyed (or created) while the second type is the radiation processes (R-processes) in which a magnon is created (or annihilated) and a magnon and a phonon are destroyed (or created). They represented these types of interactions by relaxation times in the phonon scattering mechanism while the contribution of magnons to the heat current was neglected.

Mikhail et al. [27] performed a detailed study of thermal conduction in antiferromagnets where the contributions of magnons and phonons to the thermal scattering and thermal current were taken into account. They started by the two transport Boltzmann equations of phonons and magnons. The magnon–phonon interactions were described in detail in terms of the two magnon–one phonon C and R processes introduced in Dixon [34] and Dixon et al. [35]. Both Normal and Umklapp processes were taken into consideration. The resulting collision operator of magnon–phonon interactions has consequently been replaced for Normal and Umklapp processes by a model operator which possesses the same important properties as the exact operator. The other scattering processes were treated as resistive processes by using the relaxation time approximation. This technique may not be suitable to deal with three-phonon interactions since it does not take into consideration the effect of the wavevector conservation and quasi-conservation that occur respectively in the Normal and Umklapp processes of this type of phonon interactions. As a result the expression for thermal conductivity derived in Mikhail et al. [27] did not involve terms that correspond to the second term of the Callaway model [36] and to the modification considered in Mikhail [37]. In view of this it was felt that the three-phonon Normal and Umklapp interactions have to be dealt with in a more accurate manner. This is the aim of the present work.

In the present work the three-phonon interactions are taken into consideration by using an approach in which the conservation conditions are preserved. Alternative techniques were used by Hamilton [38], Simons [39,40], Srivastave [41] and Mikhail and Madkour [42]. Simons [40] introduced a model operator which has the advantage that it possesses the same important properties as the exact collision operator. It satisfies the conservation of the wavevector in the three-phonon Normal processes and accordingly gives rise to the second term of the Callaway expression for thermal conductivity. It was also applied in Mikhail [37] to produce an adequate modification for the thermal conductivity Callaway expression that represents the quasi-conservation of the wavevector in the three-phonon Umklapp processes. Mikhail and Madkour [42] constructed a model operator that was mainly based on the isotropic approach introduced in Parrott [43] and Hamilton and Parrott [44]. It possesses the same essential properties as the Simons Model [40]. It was also used to derive the modification that occurs in the thermal conductivity expression due to the three-phonon Umklapp processes quasi-conservation of wavevector. The relaxation times as well as the related quantities were calculated from their complicated exact expressions that depend on the third order elastic constants.

Here, the Simons model [40] will be utilized to represent the three-phonon Normal and Umklapp processes since the operators that were used in Mikhail et al. [27] to represent the magnon–phonon interactions were formulated in a similar manner. The use of the isotropic model of Mikhail and Madkour [42] has been postponed to be considered in a future article. The expression derived for thermal conductivity involves the same terms obtained in Mikhail et al. [27] that represent the contributions of magnons and phonons and the conservation conditions of magnon–phonon interactions, in addition to the required new two terms. The first of these terms stands for the second term in the Callaway expression for thermal conductivity [36] while the second represents the modification that results due to the consideration of the wavevector quasi-conservation in the three-phonon Umklapp processes. It resembles the modification terms that were derived in Mikhail [37] and Mikhail and Madkour [42].

The present work is arranged in the following way. In Section 2 the Boltzmann equations of phonons and magnons have been constructed so that the magnon–phonon C and R processes of Dixon [34] were taken into consideration. In Section 2.1 the model operator technique was used to deal with both Normal and Umklapp three-phonon interactions. The solution of the phonon linearized Boltzmann equation was accordingly derived. Section 2.2. is devoted to solve the magnon linearized Boltzmann equation by using the model operators introduced in Mikhail et al. [27]. The corresponding expression for thermal conductivity of antiferromagnetic materials has been deduced in Section 3. Finally, the application of the results to calculate the thermal conductivity of the antiferromagnet $FeCl_2$ has been performed in Section 4. The comparison of the results with the experimental measurements of Laurence and Petitgrand [24] has been displayed and the contributions due to the two new terms have been presented and discussed.

2. Boltzmann equations of phonons and magnons

The Boltzmann equation for a phonon of wavevector $\underline{q}$ and polarization σ in the presence of a temperature gradient $\underline{\nabla}T$ takes the form