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Functional crossover in the dispersion relations of magnons and phonons

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Abstract. Experimental data are presented showing that the dispersion relations of magnons and acoustic phonons can consist of two sections with different functions of wave vector. In the low wave vector range a power function of wave vector often holds over a finite q-range while dispersions for larger wave vector values better approach the atomistic model predictions. In the magnon spectra $\sim q^x$ power functions with exponents x=1.25, 1.5 and 2 are identified. The dispersion of the acoustic phonons can be a linear function of wave vector over a surprisingly large range of energy. Since the slope of the linear section agrees with the known sound velocities it can be concluded that the dispersion of the acoustic phonons has got attracted by the linear dispersion of the mass less Debye bosons (sound waves). Due to the different (translational) symmetries of bosons and atomistic excitations (magnons, phonons) the associated dispersions can attract each other. In the same way the different $\sim q^x$ power functions in the magnon dispersions indicate that magnon dispersions are attracted by the dispersion of the bosons of the magnetic continuum (Goldstone bosons). This allows evaluation of the otherwise difficult to obtain dispersions of the Goldstone bosons from the known magnon dispersions. Interestingly, the dispersions of Goldstone bosons (Debye bosons) attract magnon dispersions (phonon dispersions) and not vice versa.

1. Introduction

Since development of Renormalization Group (RG) theory it became clear that in crystalline solids one has to distinguish between two translational symmetries: the discrete translational symmetry of the atomistic lattice and the continuous translational symmetry of the infinite or continuous solid [1]. The two symmetries are the generators of distinguished particles with specific excitation spectra. Well investigated excitations of the atomistic solid are magnons and phonons. These excitations can be studied using inelastic neutron scattering. The excitations of the continuous elastic solid, the Debye bosons (=sound waves), are mass less. Mass less bosons are invisible to neutrons. The various bosons of the magnetic continuum we call Goldstone bosons [2]. Because of their different translational symmetries Goldstone bosons (Debye bosons) and magnons (acoustic phonons) can be anticipated to interact weakly only. Interactions between particles of different symmetry can manifest as attraction of the associated dispersion relations. This interaction is mainly for small q-values (large wavelengths). The aim of this phenomenological study is to show that due to this interaction the dispersions of magnons (acoustic phonons) can assume the dispersion of the Goldstone bosons (Debye bosons) for small q-values. Note that the dispersions of freely propagating bosons are simple power functions of wave vector over a large range of energy. In particular, for mass less bosons the dispersion is linear. As a consequence, the dispersion of magnons and acoustic phonons can start as a power function of wave vector over a finite q-range. The power function can be identified as dispersion of the field bosons. This opens the opportunity to evaluate the difficult to obtain dispersions of the Goldstone bosons (Debye bosons) from the known magnon (phonon) dispersions. At the limit of the power function crossover to a different function of wave vector occurs. Note that this type of crossover is different from the better known crossover events between different power functions of temperature either in the temperature dependence of order parameter or of heat capacity [3]. It is evident that atomistic spin wave theory (lattice theory) can give correct description of the magnon dispersions (phonon dispersions) only if interactions with Goldstone bosons (Debye bosons) are negligible. Obviously, in the low wave vector range field theories are necessary to explain the different exponents

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x of the ~q^x power functions. When interactions between atomistic excitations and bosons are large, the power function holds over a relatively large q-range. For larger wave vector values the dispersion of magnons and acoustic phonons is determined essentially by inter-atomic interactions. In this q-range atomistic theories appear to be appropriate. In other words, atomistic theories and field theories are complementary and have to be applied to different parts of the observed atomistic excitation spectra.

There is, however, a fundamental difference between Goldstone boson field and Debye boson field. The Debye boson field is a scalar or isotropic field. The dispersion of the Debye bosons is a linear function of wave vector along all crystallographic directions. The sources of the Debye field quanta therefore must be spherical objects. Possibly these are the nearly spherical atomic cores. The Goldstone boson field is a vector field and can have different dispersions along different crystallographic directions. The vector character of the Goldstone boson field is a consequence of the axial generation process of the field quanta by precessing magnetic moments. The Goldstone bosons are essentially magnetic dipole radiation emitted upon precession of the ordered moments [4]. Since integer and half-integer spins precess differently they generate different types of field quanta. The properties of the Goldstone boson fields therefore are different in magnets with integer and half-integer spin. Because emission of magnetic dipole radiation is by stimulated emission the basic boson field is one-dimensional and much resembles the radiation field of a LASER. This is realized in each magnetic domain. The one dimensional field aligns all spins along its axis irrespective of local exchange anisotropies. Stimulated emission of the Goldstone bosons is the origin of perfectly collinear spin structures.

Here we focus on the peculiar phenomenon that in non cubic magnets the dispersion of the Goldstone bosons can be a different power function of wave vector along different crystallographic directions. Formally we have to attribute different field dimensions to the different ~q^x power functions. In other words, three exponents x can be expected to occur in magnets with integer and in magnets with half-integer spin, respectively (see table 1). Note that for any ~q^x dispersion relation the heat capacity of the boson field follows universal T^ε power function. In other words, the exponents ε and x are correlated. For the Debye boson field only x=1 and ε=3 occur. It is evident that only one of the observed ~q^x power functions can be the relevant excitation to define the global dimensionality of the bulk magnet. The global dimensionality can be noticed from the exponent ε observed either in the thermal decrease of the order parameter or in the thermal increase of the magnetic heat capacity [5]. Note that thermal decrease of the magnetic order parameter is controlled by the heat capacity of the Goldstone boson field. Obviously there exists a complicated symmetry selection rule for the global ~q^x dispersion of the bulk magnet. In RG theory it is customary to call this selection rule relevance [1]. Another difference between the Goldstone boson field and the Debye boson field is that in insulating solids the Debye boson field is the relevant excitation spectrum for temperatures below ~10…15 K only. Relevant means that the heat capacity of the solid is the heat capacity the Debye boson field, and follows universal T^3 function in all solids. Note that universality i.e. independence of lattice structure is the characteristic thermodynamic behavior of a field of freely propagating bosons. Typical for boson dynamics is that the critical power functions hold over a finite distance from critical temperature. Note that the atomistic critical power functions hold asymptotically only. For larger temperatures than crossover at ~10…15 K phonons are the relevant excitations. The dynamics then is lattice specific. Quite generally, boson fields are the relevant excitations in the vicinity of critical temperatures (stable fixed points). In diamagnets there is only one stable fixed point at T=0. In ordered magnets there are two stable fixed points at T=0 and at $T=T_c$. The validity range of the two associated critical power functions is large. The two power functions overlap and give complete description of the magnetic order parameter for all temperatures in the ordered state [3]. As a consequence, in the ordered state the dynamics (of the spins) is entirely determined by the boson guiding field. The magnetic part of the heat capacity is that of the Goldstone boson field. Magnons are non-relevant excitations and do virtually not contribute to the magnetic heat capacity.

2. Interactions between magnons and Goldstone bosons

As we have explained elsewhere [5] the magnon excitation gap is a direct measure of the interaction strength between magnons and Goldstone bosons. Condition for direct interactions between magnons and Goldstone bosons is that the Goldstone bosons have magnetic moment. The bosons therefore must have mass, and the dispersion cannot be linear. Only for the magnets with isotropic boson field and half-integer spin the dispersion of the Goldstone bosons is a linear function of wave vector [6]. These bosons are mass less and cannot have magnetic moment. In fact, there is virtually no magnon gap observed for this class of magnets [3]. It is evident that spin wave theory can give correct description of magnon dispersions only for a vanishing magnon-Goldstone boson interaction. In other words, spin wave theory has problems in explaining a magnon excitation gap, in particular in isotropic magnets with pure spin moments. For magnets with a sizeable magnon gap the continuous part of the magnon dispersion initially also is determined by magnon-Goldstone boson interactions and follows over a finite q-range a single power function of wave vector. The q-range of the power function is the larger the larger the interaction, i.e. the magnon gap is. The observed power function can be identified with the dispersion of the Goldstone bosons. Prominent example to prove this is MnF_2 [7-9]. In MnF_2 the Goldstone boson field is along tetragonal c-axis. Spin order in bulk MnF_2 is as for a single magnetic domain. The one-dimensional boson field aligns all Mn^{2+} moments rigidly along its axis, the crystallographic c-axis. The spin-flop field is as large as ~120 kOe [10]. This anisotropy field is much too large to be explained by atomistic models. Considering the pure spin moment of the Mn^{2+} ion and the isotropic magnon dispersions [8, 9] the spin flop field should be smaller by at least a factor of 100.

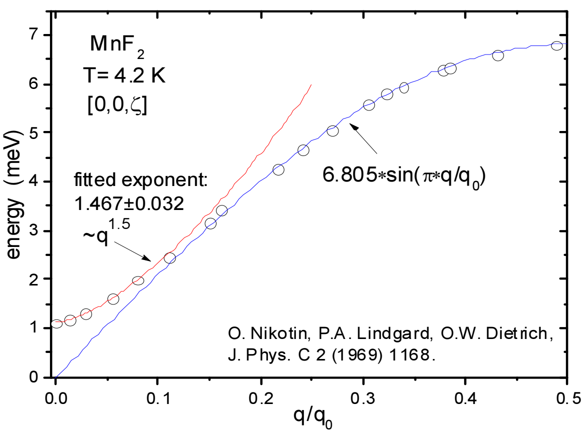

Figure 1. Functional crossover in the magnon dispersion curve of MnF_2 along tetragonal c-axis [8]. For small wave vector values magnon dispersion is given by gap value plus $q^{1.5}$ power function. The $q^{1.5}$ dispersion is that of the one-dimensional Goldstone boson field in magnets with half-integer spin (S=5/2). For larger wave vector values magnon dispersion is excellently described by sine function of wave vector.

At Néel transition only the z-components of the Mn^{2+} moments order [7]. This shows that the magnetic phase transition is executed by the one-dimensional boson field and not by the isotropic exchange interactions. MnF_2 therefore has to be classified as a one-dimensional antiferromagnet. Knowing that the boson field is one-dimensional in MnF_2, the $q^{1.5}$ power function observed in the low q-range of the magnon dispersion along c-axis (figure 1) can be interpreted as dispersion of the one-dimensional boson field in magnets with half-integer spin (S=5/2). This conclusion is consistent with investigations of the dispersion relations of resonating boson states in thin ferromagnetic films [6]. It is important to note that the standing magnetic wave experiments on metallic ferromagnetic films are a completely different and independent experimental method.

The uranium monopnictides nominally are cubic but undergo weak lattice distortions as a function of decreasing temperature. In USb the effective spin is $S_{eff}=1$ according to an observed saturation magnetic moment of $m_s=2.73\pm0.05$ μ_B/U [11]. Integer spin is consistent with $T^{9/2}$ function observed in the temperature dependence of the antiferromagnetic order parameter [12]. However, with decreasing temperature, lattice distortions increase monotonously and, eventually, become relevant. This happens at crossover temperature of $T_{CO}=105$ K where the temperature dependence of the order parameter changes from $T^{9/2}$ function to T^2 function. The T^2 universality class belongs to the three-dimensional but anisotropic boson field in magnets with integer spin. In inelastic neutron scattering measurements performed at T=10 K $\sim q^{1.5}$ and $\sim q^{1.25}$ power functions of wave vector can be identified along different crystallographic directions (figure 2). As systematic analyses of inelastic neutron scattering spectra of many other magnets show [5] the $\sim q^{1.5}$ power function is the dispersion of the one-dimensional boson field but the $\sim q^{1.25}$ function is the dispersion of the three-dimensional but anisotropic boson field in magnets with integer spin. Observation of T^2 function in the order parameter of USb (at T=10 K) shows that the $\sim q^{1.25}$ dispersion is the relevant excitation for $T<T_{CO}$. If $\sim q^{1.5}$ function would be relevant the order parameter would follow T^3 function (see table 1). On the other hand it can be expected that for $T>T_{CO}$=105 K where the order parameter follows isotropic $T^{9/2}$ function, $\sim q^2$ dispersion appears in the magnon spectrum. It is typical that the boson defined part of the magnon dispersions depends sensibly on mesoscopic parameters such as weak lattice distortions. The exchange defined part of the magnon spectrum at larger wave vector values is more stable against weak lattice distortions.

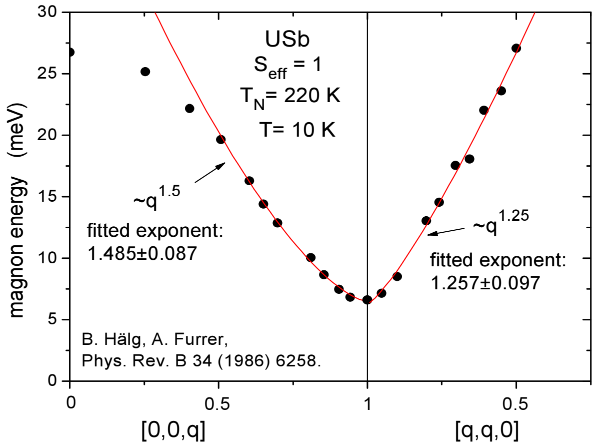

Figure 2. Magnon dispersions of antiferromagnetic USb measured at T=10 K along two crystallographic directions [11]. Along cube edge dispersion of the Goldstone bosons is $\sim q^{1.5}$ while along face diagonal $\sim q^{1.25}$ dispersion holds. The $\sim q^{1.25}$ dispersion is consistent with T^2 dependence observed below T_{CO}=105 K for the magnetic order parameter (see text).

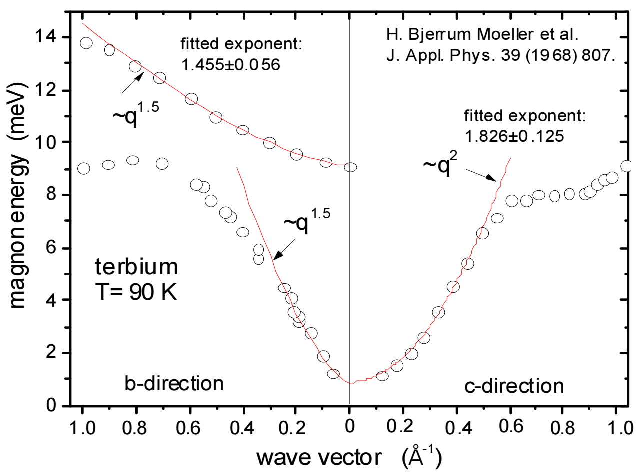

Figure 3. Magnon dispersions of terbium along hexagonal c-axis and transverse to c-axis (along b-direction) [13]. Assuming integer moment of J=6 according to electronic configuration of $^7F_6$ of the Tb^{3+} ion, $\sim q^2$ dispersion is typical for the isotropic boson field but $\sim q^{1.5}$ dispersion for the one-dimensional boson field in magnets with integer spin.

Hexagonal terbium has been extensively studied using inelastic neutron scattering [13, 14]. In the magnon spectra of [13] $\sim q^2$ dispersion can be identified along hexagonal c-axis. Transverse to c-axis $\sim q^{1.5}$ dispersion holds with high precision (figure 3). Interpretation of the two dispersion functions becomes, however, not clear considering terbium alone. Assuming that crystal field interaction is not relevant and that the full integer moment of J=6 of the configuration $^7F_6$ of the Tb^{3+} ion holds, the two power functions of wave vector are characteristic for magnets with integer spin. In fact, $\sim q^2$ function is the dispersion of the isotropic boson field and $\sim q^{1.5}$ function is the dispersion of the one-dimensional boson field in magnets with integer spin. Final interpretation of the observed $\sim q^x$ dispersion relations must come from magnets with stable magnetic moments and crystal structures that allow definite conclusion on the dimensionality of the boson field [5].

UO_2 is another nominally cubic crystal with integer spin of S=1 that undergoes weak lattice distortion as a function of decreasing temperature. Lattice distortions can be sample dependent. The usually large single crystals used in inelastic neutron scattering studies frequently are strongly strained. As we now know, the Goldstone boson field depends sensitively on lattice deformations. Axial strain in cubic magnets can reduce the dimensionality of the Goldstone boson field from isotropic to one-dimensional. In the magnon dispersions of the large UO_2 single crystal (2x2x4 cm) investigated in [15] dispersions as $\sim q^{1.5}$ can be identified along body diagonal (figure 4). Along cube edge $\sim q^{1.25}$ is observed (figure 5). For perfect cubic lattice symmetry $\sim q^2$ should be observed along all crystal directions. As a consequence, the UO_2 crystal investigated in [15] was not perfectly cubic.

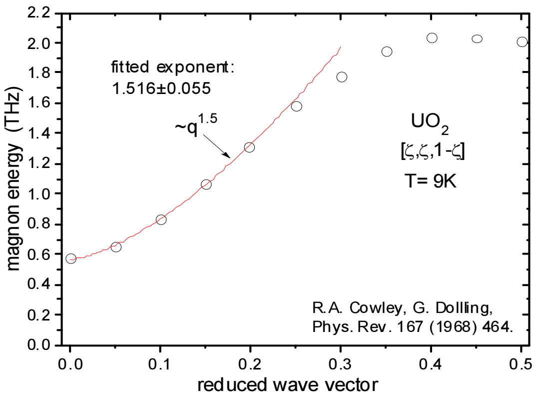

Figure 4. Magnon dispersions of nominally cubic UO_2 along body diagonal [15]. The observed $\sim q^{1.5}$ dispersion is that of the one-dimensional boson field in magnets with integer spin (S=1). This UO_2 sample was not perfectly cubic.

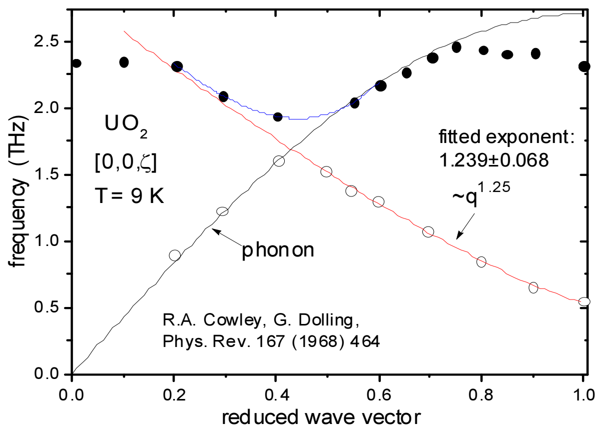

Figure 5. Magnon dispersions of UO_2 along cube edge revealing $\sim q^{1.25}$ dispersion [15]. This dispersion is attributed to the anisotropic 3D boson field in magnets with integer spin (S=1).

In the magnon dispersions of orthorhombic $LaMnO_3$ (figure 6) dispersions as $\sim q^{1.5}$ and q^2 can be identified. According to an observed saturation magnetic moment of m_s=3.87 μ_B/Mn the spin of the

Mn^{3+} ion is S=2 [16]. Since T^3 dependence can be identified in the magnetic order parameter [16] the $\sim q^{1.5}$ excitation spectrum seems to be relevant for the thermodynamics of the three-dimensional solid.

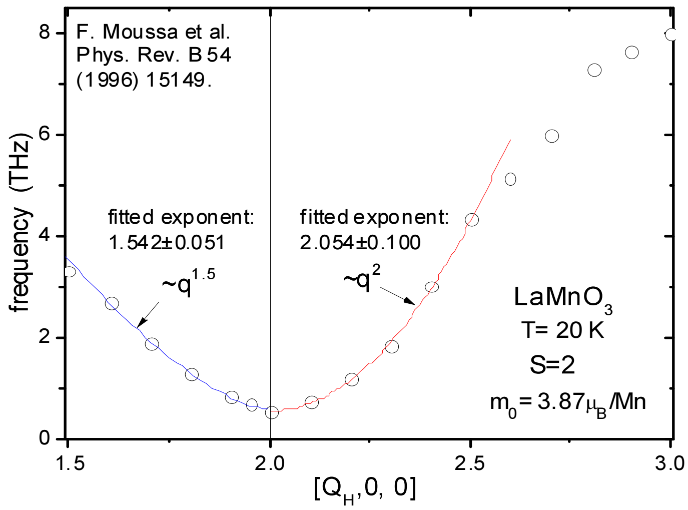

Figure 6. Magnon dispersions of orthorhombic $LaMnO_3$ with integer spin of S=2 [16]. The dispersion $\sim q^2$ is attributed to the isotropic boson field in magnets with integer spin. The dispersion $\sim q^{1.5}$ belongs to the one-dimensional boson field.

As a summary of our studies table 1 compiles the temperature power functions for the heat capacity of the boson fields and the associated dispersion relations in dependence of the dimension of the field (d) and spin quantum number.

Table 1. Power functions of temperature (T^ε) and of wave vector (q^x) for heat capacity and dispersion relation of the Goldstone boson field, respectively, in dependence of field dimensionality (d) and spin quantum number. The T^ε functions apply equally to the thermal decrease of the magnetic order parameter.

field dimensionality	integer spin	half-integer spin
d=3	$T^{9/2}$; q^2	T^2; q
d=2	T^2; $q^{1.25}$	$T^{3/2}$; q^2
d=1	T^3; $q^{1.5}$	$T^{5/2}$; $q^{1.5}$

3. Interactions between Debye bosons and acoustic phonons

For freely propagating sound waves (Debye bosons) the dispersion is a linear function of wave vector for all energies. However, interactions with the atomistic background of phonons and lattice imperfections provide damping to the Debye bosons. Sound velocities and elastic constants therefore depend somewhat on sample quality. Damping shortens the mean free path of the sound waves and decreases their velocity. In fact, sound velocities commonly decrease as a function of increasing temperature [17]. As a consequence the dispersion of the Debye bosons increases slightly weaker than linear.

Interactions between acoustic phonons and Debye bosons usually are stronger for longitudinal polarization than for transverse polarization. In AgBr these interactions are particularly strong. The longitudinal phonon branch initially is a linear function of wave vector up to energy of 2THz (~96 K) (figure 7) [18]. At this thermal energy the dispersion of the Debye bosons is no longer populated and phonons are the relevant excitations. It therefore can be concluded that the acoustic phonons can get attracted by the non populated Debye boson dispersion. This allows verification of the dispersion of the Debye bosons from phonon dispersion up to surprisingly high energies. Since the slope of the linear section agrees with the measured sound velocity [19] it becomes evident that phonon dispersion has been attracted by the dispersion of the Debye bosons. It is evident that the dispersion of the Debye bosons must continue up to much higher energies than the linear section in the phonon dispersion. For transverse polarization phonon data follow with good accuracy sine function of wave vector. However, in order to get correct description of the experimental data it is necessary to add a phase shift to the argument of the sine function. As a consequence, phonon-Debye boson interactions are noticeable all over the Brillouin zone. This seems to be different for the magnon dispersions (figure 1). Unfortunately no phonon data were measured along linear dispersion of v_T.

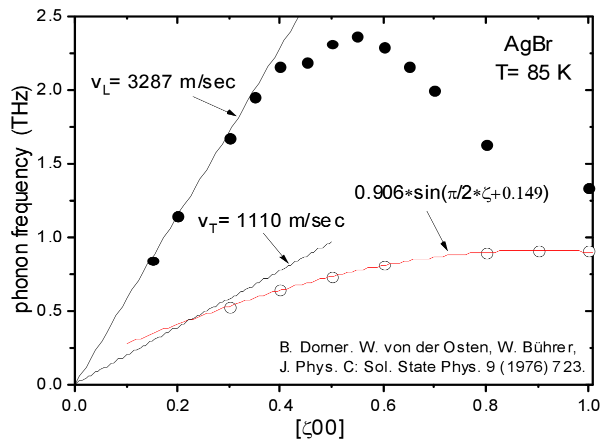

Figure 7. Dispersions of the acoustic phonons with longitudinal and transverse polarization of AgBr [18]. For longitudinal polarization the dispersion of the acoustic phonons agrees with the dispersion of the Debye bosons (sound waves) up to ~2 THz (~96 K). For transverse polarization interaction with Debye bosons necessitates a phase shift in the argument of the sine function.

3. Conclusions

Since development of RG theory it became clear that the continuous translational symmetry of the infinite solid is a particle generating symmetry. Critical dynamics is due to these particles. Sound waves (Debye bosons) are the particles or excitations of the elastic continuum. The particles of the magnetic continuum we have called Goldstone bosons [2]. The excitations of the continuous solid exist in addition to the excitations of the atomistic solid. The two excitations define the dynamics alternatively. Change of dynamics from one excitation spectrum to the other is a crossover. A crossover is a symmetry change. As a consequence, in magnetic solids one has to distinguish between four excitation spectra. Prominent particles or excitations of the atomistic solid are magnons and phonons. In spite of different translational symmetries Debye bosons and Goldstone bosons can interact with the atomistic excitations. These interactions can be surprisingly strong for large wavelengths. In the present communication we have focused on interactions between Goldstone bosons and magnons and on interactions between Debye bosons and acoustic phonons. Debye bosons can interact also with magnons; Goldstone bosons can interact also with phonons. Due to their different symmetries the dispersions of bosons and atomistic excitations can attract each other. Note that the dispersions of particles with identical symmetry avoid each other. It turned out that the dispersions of the bosons attract the dispersion of the atomistic excitations and not vice versa. In other words, for small wave vector values the dispersions of magnons and acoustic phonons assume the dispersion of Goldstone bosons and Debye bosons, respectively. This allows evaluation of the difficult to obtain dispersion relations of the bosons from the known inelastic neutron scattering spectra of the atomistic excitations of magnons and phonons. The Debye boson field is a scalar or isotropic field. There is no preferential field direction. The Goldstone boson field is a vector field and can assume any dimension. The vector character of the Goldstone boson field is a consequence of the axial generation process of the field quanta by precessing spins [4]. Goldstone bosons are essentially magnetic dipole radiation. Essential for the one dimensional Goldstone boson field is that magnetic dipole radiation is generated by stimulated emission. Collinear spin alignment in all magnetic domains is along direction of the boson field. However, coupling of the one-dimensional field components of the individual domains to result into an isotropic field of the bulk magnet is a completely unexplored process.

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