

Spin dynamics of half-metallic Co_2MnSi

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Abstract. Spin dynamics of half-metallic Co_2MnSi is studied using linear response density functional theory. The material features three well defined spin-wave branches. Since the half-metallicity implies a finite activation energy for the Stoner states the low energy magnons cannot decay via Landau mechanism.

1. Introduction

An important class of materials for spintronics applications are half-metals, especially Heusler phases [1, 2]. In these complex systems one of the spin channels is semi-conducting, while the other is metallic. A substantial effort has been devoted to the study of spin-flip excitations in Heusler alloys, since the excitations determine the temperature dependence of magnetic properties, the Curie temperature and can influence the operation of ever smaller and faster spintronic devices. In a ferromagnetic system there are two major mechanisms leading to a change of net magnetic moment. First is the single-electron spin-flip (Stoner) excitation, in which an electron is promoted from an occupied state with a given spin projection to an empty state with an opposite spin projection. The second type are so called spin waves (SW), which are collective excitations of the electron system often visualized as a coherent precession of atomic moments. The SWs can hybridize with Stoner excitations, which leads to so called Landau damping. This is the dominating SW decay channel in metallic magnets. In half-metals the Stoner excitations acquire a finite activation energy γ_S equal to the difference of the bottom of the conduction band and the Fermi energy. For magnons with energies below γ_S the Landau decay is impossible.

In this paper we focus on the spin dynamics of half-metallic Co_2MnSi , material of particular importance in the spintronics [3]. This example allows us to explore the interplay between the half-metallicity and spin excitations. Additionally, several magnetic sublattices of Co_2MnSi give us a chance to study the formation of optical magnons. Sec. 2 outline briefly the formalism of the linear response density functional theory (LRDFT), which allows to address the SWs and Stoner states on an equal footing starting from first principles. Sec. 3 describes our results.

2. Formalism

The magnetic susceptibility determines the spectrum of spin excitations of a system and LRDFT [4] allows to determine the quantity in a parameter free manner. The details of the formalism for collinear magnets [5] and the details of our computational implementation [6] can be found elsewhere. Briefly, two types of response functions are considered: the Kohn-Sham (KS) (unenhanced) susceptibility χ_{KS} and the true (enhanced) susceptibility χ . The first one carries information about the Stoner continuum, while the second contains in addition the SW excitations.

The retarded KS susceptibility is constructed based on the self-consistent KS eigenfunctions and eigenenergies (φ_k and ϵ_k respectively)

$$\chi_0^{ij}(\mathbf{x}, \mathbf{x}', \omega) = \sum_{km} \sigma_{\alpha\beta}^i \sigma_{\gamma\delta}^j (n_k - n_m) \frac{\varphi_k(\mathbf{x}\alpha)^* \varphi_m(\mathbf{x}\beta) \varphi_m(\mathbf{x}'\gamma)^* \varphi_k(\mathbf{x}'\delta)}{\omega + \epsilon_k - \epsilon_m + 0^+}, \quad (1)$$

where $i, j = x, y, z$, $\boldsymbol{\sigma}$ stands for the vector of Pauli matrices. The ground state magnetization is assumed to point along z direction. n_k is 1 if ϵ_k is smaller than the Fermi energy and 0 otherwise.

If one casts the spatial and ij dependence of the susceptibility matrices into a suitable basis, the enhanced susceptibility can be found from the following equation

$$\chi(\omega) = (1 - \chi_{\text{KS}}(\omega) K_{\text{xc}})^{-1} \chi_{\text{KS}}(\omega). \quad (2)$$

The exchange correlation kernel K_{xc} takes into account the self-consistent change of the electronic environment in the presence of the oscillating external field. $\chi(\omega)$ can develop a singularity outside the Stoner continuum, providing the matrix $1 - \chi_{\text{KS}}^{ij}(\omega) K_{\text{xc}}$ becomes singular for certain frequency. This new type of excitations are SWs.

In the case of the translationally invariant systems the susceptibility can be written as $\chi(\mathbf{r}, \mathbf{r}', \mathbf{q}, \omega)$, where \mathbf{r} and \mathbf{r}' are vectors in the Wigner-Seitz cell Ω and \mathbf{q} belongs to the first Brillouin zone of the crystal. For every \mathbf{q} the eigenvectors and eigenvalues χ_λ (λ labels the eigenvalues) of $\chi(\mathbf{r}, \mathbf{r}', \mathbf{q}, \omega)$ matrix determine the SW modes of the system. The frequency dependence of χ_λ is well described by a Lorentzian

$$\chi_\lambda(\mathbf{q}, \omega) \approx \frac{A_\lambda(\mathbf{q})}{\omega - \omega_{0\lambda}(\mathbf{q}) + i\beta_\lambda(\mathbf{q})}, \quad (3)$$

where $\omega_{0\lambda}$ is the SW energy, while β_λ can be interpreted as the inverse life-time of the state.

The cross section in a magnetic inelastic neutron scattering experiment is proportional to the imaginary part of the Fourier transform of the susceptibility [7]

$$\chi^{xx}(\mathbf{q} + \mathbf{K}, \omega) = \chi^{yy}(\mathbf{q} + \mathbf{K}, \omega) = \iint_{\Omega^2} d\mathbf{r} d\mathbf{r}' e^{-i(\mathbf{q}+\mathbf{K}) \cdot \mathbf{r}} \chi^{xx}(\mathbf{r}, \mathbf{r}', \mathbf{q}) e^{i(\mathbf{q}+\mathbf{K}) \cdot \mathbf{r}'}, \quad (4)$$

where \mathbf{K} is a vector of the reciprocal lattice. $\mathbf{q} + \mathbf{K}$ is the neutron momentum loss.

3. Results

The half-metallic gap in Heusler compounds arises due to the hybridization of electronic $3d$ states of the transition metal atoms and the mechanism is well understood [1]. According to our estimates the half-metallic gap amounts to 14.6 mRy, but the Fermi energy is located close to the bottom edge of the conduction band and therefore the activation energy γ_S for Stoner excitations is only about 3.8 mRy. The tunneling magnetoresistance experiments [3] yield qualitatively similar picture of electronic structure around the Fermi energy, but much smaller $\gamma_S \approx 0.7 \div 1.5$ mRy and larger half-metallic gap of about 29 mRy.

The spectral density of the Stoner continuum in the SW energy range is presented in the Fig. 1. It becomes pronounced only above 40 mRy, but low energy Stoner excitations can be found with energies down to γ_S . As shown in the Fig. 3, the bottom edge of the Stoner continuum depends strongly on \mathbf{q} . The Stoner states are more localized in the energy space near the Γ point in the Brillouin zone, which places the edge at higher energy.

Fig. 2 presents the energy dependence of blocks $\chi_{\text{KS}}^{ab}(\mathbf{q}, \omega)$ ($a, b = \text{Mn, Co}$) of Kohn-Sham susceptibility corresponding to the magnetic coupling between different magnetic sublattices

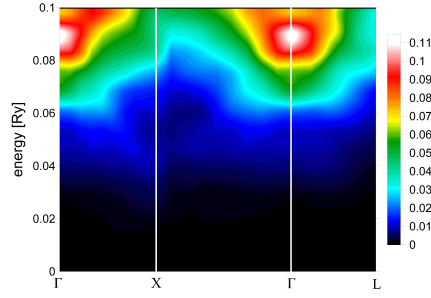


Figure 1. Spectral density of Stoner excitations, $\Im\chi_{KS}(\mathbf{q}, \omega)$, along the high symmetry directions in the Brillouin zone. $\Im\chi_{KS}(\mathbf{q}, \omega)$ becomes pronounced above 40 mRy, leading to the attenuation of the optical SW modes. The bottom edge of the spectrum is presented in Fig. 3.

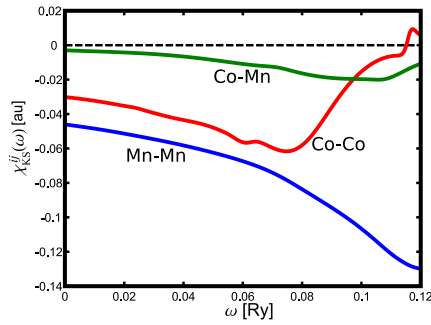


Figure 2. The energy dependence of the blocks of KS susceptibility, corresponding to the magnetic coupling between different magnetic sublattices. The figure correspond to $\mathbf{q} = 0.28(1, 1, 0)\frac{2\pi}{a}$.

for a selected momentum transfer. χ_{KS}^{ab} describes the non-selfconsistent magnetization induced on the sublattice a when spin spiral magnetic field is applied to sublattice b . We notice that the diagonal atomic blocks (i.e. the blocks describing the coupling within the given magnetic sublattice) dominate over the off-diagonal ones (representing the interlattice coupling). Since the kernel K_{xc} is frequency independent and rather similar for different $3d$ elements, the formation of SW is primarily controlled by $\chi_{KS}^{aa}(\mathbf{q}, \omega)$. If only the diagonal atomic blocks were retained we would obtain the dynamics of decoupled magnetic sublattices. In this case the SWs would not disappear, i.e. every magnetic sublattice is capable of maintaining its own SW branch. The off-diagonal blocks lead to the hybridization of the branches influencing the energies and the shapes of the SW excitations, but upon their removal the number of SW modes does not change.

Despite the damping of SWs, Co_2MnSi can still be regarded as well defined excitations. Their energies and inverse life times are presented in the Fig. 3. The lowest mode (“acoustic” or EV 1) has vanishing energy for $\mathbf{q} = \mathbf{0}$. This is a manifestation of the spin rotational invariance of the system in the case of neglected magnetic anisotropy. As expected, the width of EV 1 peak is zero within the numerical noise when the SW appear in the gap of the Stoner continuum. Additionally we note that $\beta_1(\mathbf{q})$ does not exceed 0.37 mRy even above the edge of Stoner continuum, where the Landau damping is in principle not excluded. The negligible attenuation is a natural consequence of the small spectral density of Stoner excitations in this region. On the contrary, the “optical” modes (EV 2 and 3) appear where the continuum density is not small and therefore have significant width, which depends strongly and non-monotonously on \mathbf{q} , Fig. 3b.

The number of SW modes corresponds to the number of magnetic atoms in the primitive cell and therefore Co_2MnSi – up to the damping – is a typical Heisenberg Hamiltonian system. In the EV 1 mode the atomic moments oscillate in phase, roughly given by $e^{i\mathbf{q}\cdot\mathbf{r}_i}$, where \mathbf{r}_i stands for the position of atom i . For the optical modes some of the moments align themselves roughly in the anti-phase to the others.

It is not very likely that the optical modes could be experimentally detected in typical neutron scattering experiments. First, they are very energetic and are substantially damped. Second, it

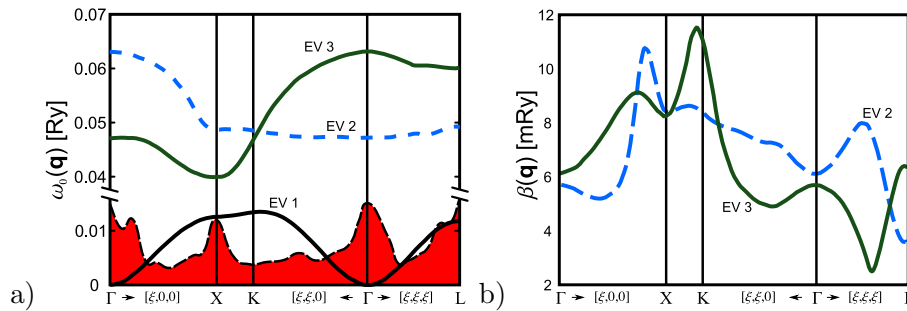


Figure 3. Energies (a) and inverse life-times (b) of three SW modes in Co_2MnSi . The lowest mode (EV 1) has maximum energy of 13.5 mRy around point K. It is separated by a gap of around 27 mRy from the optical modes EV 2 and EV 3. Parameter $\beta_1(\mathbf{q})$ of EV 1 does not exceed 0.37 mRy and it is not shown. The Stoner excitations cannot appear in the shaded \mathbf{q} - ω region of panel a) and the dashed line (---) marks the bottom edge of their spectrum.

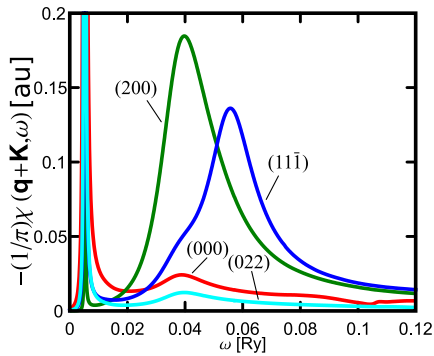


Figure 4. The imaginary part of Fourier transformed susceptibility of Co_2MnSi for $\mathbf{q} = 0.28(1, 1, 0)\frac{2\pi}{a} + \mathbf{K}$. The triples of numbers represent \mathbf{K} in units of $2\pi/a$. Different optical branches can be resolved only well outside the 1st BZ, while the optical peak is always present.

is impossible to probe them at small momentum transfers. Fig. 4 presents an example of the imaginary part of the Fourier transformed susceptibility. While the acoustic peak is present (with different intensity) for every \mathbf{K} , the optical branches could be resolved only for extremely large momentum transfers. The behavior can be understood when we realize that the projection of an optical mode on a long wave-length plane wave $e^{i\mathbf{q}\cdot\mathbf{r}}$ is necessarily small, since the contributions from the moments oscillating in the antiphase cancel each other.

In summary, we presented the LRDFT study of magnetic excitations of half-metallic Heusler phase Co_2MnSi . The system features three SW modes, corresponding to three well defined magnetic sublattices. The finite activation energy of Stoner states makes the Landau damping of SWs ineffective at low energies. For this reason half-metals at low temperatures give a chance to study of than Landau-type decay mechanisms and fine effects like coupling of magnons to phonons and electronic degrees of freedom. The optical magnons are substantially attenuated because of the hybridization with the single-particle excitations. In neutron scattering experiments these magnons can be resolved only outside the first Brillouin zone.

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