Magnetization dynamics in disordered Fe$_x$Co$_{1-x}$ alloys: A first-principles augmented space approach and atomistic spin dynamics simulations

Banasree Sadhukhan$^\dagger$, Raghuveer Chimata$^\ddagger$, Biplab Sanyal$^{1,*}$ and Abhijit Mookerjee$^{*1}$

1$^*$Department of Physics, Presidency University, 86/1 College Street, Kolkata 700073, India.
2$^\dagger$Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden.
3$^*\ddagger$Professor Emeritus, Department of Condensed Matter and Materials Science, S.N. Bose National Centre for Basic Sciences, JD-III, Salt Lake, Kolkata 700098, India.

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In this paper, we present a general method to study magnetization dynamics in chemically disordered alloys. This computationally feasible technique, which seamlessly combines three approaches: the density functional based linear muffin-tin orbitals (LMTO) for self-consistently obtaining a sparse Hamiltonian; the generalized recursion method to obtain the one and two-particle Green functions and augmented space approach to deal with disorder averaging. The same formalism applied to both spectral and response properties should make the errors compatible in different studies. We have demonstrated a successful application to the binary chemically disordered Fe$_x$Co$_{1-x}$ alloys to explain several experimental features in magnon spectra. Our study captures significant magnon softening due to magnon-electron scattering for chemically disordered Fe$_x$Co$_{1-x}$ alloys within linear spin wave regime. As a complementary study, we have done atomistic spin dynamics simulations by solving Landau-Lifshitz-Gilbert equation with parameters obtained from ab initio multiple scattering theory to compare with the results obtained from augmented space approach.

I. INTRODUCTION.

The dynamics and damping of magnetic excitations play a pivotal role in many modern spintronic applications. From the time commercial hard-disk drives became available, their recording densities have spectacularly increased by more than seven orders of magnitude with continuous development of areal density in the magnetic recording media. High areal density has been achieved by a scaling of the dimensions of the bits recorded in the storage medium. However, the density has an upper limit. The reduction of grain size, which leads to larger areal densities makes the systems more susceptible to thermal and chemical fluctuations. The consequent super-paramagnetic effects and instabilities due to scattering processes lead to a decrease in the ratio of magnetic energy per grain $E_u V$ (where $E_u$ is the uniaxial magneto-crystalline anisotropy energy and $V$ is the grain volume), to the thermal energy $k_B T$. Retaining the magnetization of the medium over a long period of time despite thermal fluctuations is therefore, a major problem in designing magnetic storage media. In addition to large uniaxial magneto-crystalline energies and saturation magnetizations ($M_s$), another important issue in magnetic recording applications is the magnetic switching time, which imposes physical limits on data rates and areal recording densities. In this regard, a thorough understanding of the magnetization dynamics in presence of several microscopic scattering processes in technologically important alloys is essential.

In this article, we would like to examine the effects of different kinds of scatterings, in particular scattering due to chemical disorder, on the softening of magnonic branches in magnetic alloys$^{1,2}$. Theoretically a magnon has an infinite lifetime at low temperatures. But in a realistic case, damping of low energy spin-wave excitations arises from different direct scatterings between magnons and electrons, and between magnons. There are also indirect processes, which include magnon scattering with both fast- and slow-relaxing impurities, where each process has a different relaxation time. Safonov et al. have shown that both direct and indirect loss mechanisms involve non-linear oscillator excitation. This non-linear magnetic excitation gives an effective magnetization damping parameter $\alpha$ which is about 100 times greater than that in the linear regime of Landau-Lifshitz-Gilbert (LLG) damping. Both in the direct and indirect processes, scattering loss can be enhanced by chemical disorder. These impurity ions are assumed to relax at a very high rate because of spin-orbit coupling. Impurity magnetic ions of transition and rare-earth elements with strong spin-orbital coupling give rise to ferromagnetic resonance line broadening. The ‘fast-relaxing ion’ mechanism is effective when the transverse relaxation rate of the impurity is so fast that the magnetization oscillations can excite direct transitions between impurity levels. According to recent ferromagnetic resonance experiments in ultra thin films, spin wave scattering on the surface impurity is a possible mechanism of damping of the magnetization. Thus in the simulations of magnetization reversal by spin-wave dynamics, the impure magnonic damping allows the high wavelength magnons to relax faster than those with high wave-vector (Stoner damping). This plays an important role in designing mono-dispersed magnetic nano particle recording media.

Spin-wave damping is another important factor. In the ultra-fast laser induced magnetization reversal processes at high temperatures, spin wave damping is mainly governed by the Stoner continuum. To increase the areal density in magnetic recording media we need high $E_u$ materials, which also have large saturation magnetization $M_s$. In addition, substantial spin wave damping
at low temperatures is desired. At low temperatures, a spin wave damps through different scattering mechanisms. The physical sizes of the recording devices and the switching speeds have reached a point where dynamical response of magnetic system have become relevant. At high temperatures the decay of spin-wave excitations into the Stoner continuum is described successfully by the LLG equation in several aspects. The phenomenological damping employed to describe magnetization dynamics in LLG theory comes from the random force of thermal fluctuations. However, it fails to describe spin-wave excitation at lower energies where damping is governed by magnon-electron and two-magnon scattering\textsuperscript{12}.

Elementary spin-wave excitations (magnons) also play a fundamental role in many physical processes and phenomena of current research such as spintronics. The challenge of spintronics research is to explore the nature of the magnon dispersion spectrum and spin transport in pristine metals, semiconductors and their alloys. Simultaneously, the synthesis of magnons in complex low-dimensional ferromagnetic oxide nano structures has become a reality. First principles studies of spin correlation functions and magnon lifetimes of disordered magnetic systems have become important because of both fundamental and technological interest. Most theoretical studies of spin excitations to date has been employed in the classical Heisenberg model. Since the mid of 1980-s, a lot of work was done in the understanding of spin-wave interactions in systems of localized spins. This model is defined in terms of the exchange parameters, that can be obtained from constrained density-functional theory. Long-wavelength magnon excitations, i.e., spin waves with short wave vectors, can be calculated efficiently with that localized spin model. Furthermore, the Heisenberg model is not only justified for systems with localized moments, such as insulators and rare earth elements, but also for materials where the itinerant electrons are responsible for the magnetism because of the terms of density-functional based exchange interaction, which are responsible for Stoner excitation implicitly. So the Heisenberg model still yields reasonable results for large wavevector excitations in itinerant-electron magnets. To date various theoretical techniques have been employed to understand these Stoner-excitation phenomena, starting from atomic spin dynamics (UppASD)\textsuperscript{13,14} to frequency-space study of spin-wave excitations and magnons\textsuperscript{15}. Successful experiments using spin-polarized electron energy loss spectroscopy (SPEELS)\textsuperscript{14,23} unfolded an exciting scenario. But none of those theories can describe the low energy spin wave excitations fully satisfactorily and with clarity. Theoretical constructions dealing explicitly with the Heisenberg ferromagnets, include the modified spin wave theory (MSWT), the large N expansion of SU(N) Heisenberg models and Schwinger boson mean field theory (SBMFT), the self-consistent spin wave theory, renormalization group (RG) methods and mapping to lattice boson systems with additional repulsive interaction for S = 1/2. As in the earlier works had concluded that a realistic description of the low temperature phase of Heisenberg ferromagnets can be reached using bosonic (or combined bosonic-fermionic) representations of the spin operators within quartic approximation, or with the help of appropriate mean field/random phase approximations (MFA/RPA) without complicated mathematical calculation of magnon self energy. On the other hand the predictions of linear spin-wave theory (LSWT) are reliable almost up to $T_C/2$ ($T_C$ is the Curie temperature), within which we exclude the effects of magnon-magnon interactions. At low temperature magnons behave as independent boson particles. These low-energy spin wave excitations range from a few meV to a few hundreds of meV. So, they are decisive factors in the thermal and electrical transport. Thus the dynamical relaxation of various complex systems has been the focus of considerable interest. In particular, anomalous relaxation in spin glass phases has received considerable attention over the years. The analysis of the magnon excitation peak positions and broadening provides us information on the magnon energy and lifetime, respectively. Magnon energy decays exponentially like exp(-Γ/2ℏ) where Γ represents intrinsic line width of Lorentzian peak in magnon spectral density and ℏ is the reduced Planck constant. The magnon life time $\tau_0 = 2ℏ/\Gamma$ is usually defined as the time in which the amplitude drops to $e^{-1}$ of its initial value. In crystalline systems, the Floquet-Bloch theorem implies that a q labelled state is a stable quantum state, the spectral density is a bunch of delta functions at $E = E(q)$. These states have infinite life-times. In the presence of disorder or any deviation from Floquet-Bloch conditions leads to scattering, which is the origin of finite lifetimes of the q labelled quantum states.

The main objective of this work is to start from a first-principles, density functional approach with as few “parameters” as possible and shed light on the area of scattering of spin-wave excitations by both chemical disorder (impurities, doping and alloying) and structural disorder (defects, local and long-ranged deformations of the lattice). The theoretical methodology we shall use is the Recursion method of Heine et al. and the augmented space method of Mookerjee\textsuperscript{24–26}. This will allow us to forego the Floquet-Bloch conditions altogether and go beyond the mean field (coherent potential) approximations without violating the analytical conditions of the averaged propagators\textsuperscript{24–26}.

The article is organized as follows. In Sec. II we present the theoretical tools used to describe the dynamical spin response functions and the numerical details of the calculation. Sec. III contains Results and discussions. Finally, we give conclusions in Sec. IV.

II. METHODOLOGY

The behaviour which is conducive to satisfactory performance of most magnetic devices is governed by mag-
nagnetic dynamics, which is in turn regulated by damping. A phenomenological but successful model widely used is the LLG\textsuperscript{29} equation. Not surprisingly, therefore, this has led to a wide body of theoretical works on the ‘first principles’, almost parameter free, determinations of Gilbert damping from electronic structure calculations. Two successful models are the breathing Fermi surface model (BFS)\textsuperscript{30} and the torque correlation model (TCM)\textsuperscript{31}. Unfortunately, neither are the models parameter free, nor do they really shed light on the microscopic origins of damping. Finally, when it was realized that damping arose from scattering phenomena that the first truly microscopic derivations surfaced in the works of Brataas et.al\textsuperscript{32}, Starikov et.al., Liu et.al.\textsuperscript{33} and Ebert et.al.\textsuperscript{12}. The last mentioned paper identifies breakdown of Floquet’s theorem due to potential disorder as the principal cause of scattering. The breakdown can be thermal, arising from phonon-magnon scattering. Mookerjee\textsuperscript{24, 26} had introduced a formalism to describe scattering due to chemical disorder in terms of scattering by configuration fluctuations about the “average” Floquet pattern. In order to understand our later arguments we shall summarize Ebert et.al.’s argument concisely.

The LLG equation is:

\[
\frac{d\vec{m}}{dt} = -\vec{m} \times \vec{H} + \vec{m} \times \vec{V}
\]

where

\[
\vec{V} = \frac{\alpha \mu(\vec{m})}{\gamma m_s} \frac{d\mu}{dt}
\]

If \( \vec{m}(t) = \vec{m}_0 + \vec{u}(t) \), then the Hamiltonian becomes

\[
\hat{H} = \hat{H}_0(\vec{m}_0) + \vec{u} \cdot \nabla \hat{H}_0(\vec{m}_0)
\]

Now, using the expression for the dissipation energy, a Kubo-Greenwood like expression emerges:

\[
\alpha_{\mu\nu} = -\frac{\gamma}{\pi m_s} \text{Tr} \{ T_v \text{Im} m G(E_F)T_v \text{Im} m G(E_F) \}
\]

where, \( \alpha_{\mu\nu} \) is the damping parameter and \( T_v = \frac{\partial H}{\partial m_\nu} \). \( \gamma \) is the gyromagnetic ratio and \( m_s \) is the saturation magnetization.

However this does not give a complete understanding of spin wave damping and magnetization relaxation. In recent progress Bergman et.al calculated magnon dispersion spectrum on Fe/W(110) monolayer system. They showed that the strong magnon softening in that system contradicts with earlier prediction based on itinerant electron model at \( T=0 \) K. Experiments on spin-polarized electron energy loss spectroscopy (SPEELS)\textsuperscript{23-14} revealed that the magnon energies in monolayer are small compared to the bulk and surface. This discrepancy leads to the possibility that Fe/W(110) may not be a simple ferromagnet. A recent theoretical study by Grechnev et.al suggested strong electron-electron correlation leading to fast magnetization reversal and current induced magnetic switching. This has to be properly understood because of its technological application. Low dimensional magnetic system has lack of inversion symmetry and magnetic ordering comes from Dzyaloshinskii-Moriya interactions (DMI). Both of these arise from spin orbit coupling. For bulk system this effects can be ignored.

Thermal fluctuation also contributes over and above \( T=0 \) K. What is now needed a clear description of physical processes that are responsible for spin wave softening over a wide range of composition in chemically disordered alloys. Brataas et.al introduced an equivalent formulation using scattering theory and Kubo formalism for understanding this picture. The damping or the relaxation time (\( \tau_0 \)) of magnon comes from Kubo-Greenwood formalism, where damping parameter \( \alpha \propto 1/\tau_0 \). In this work we concentrate on the low temperature regime. Earlier predictions based linear spin wave theories at low temperature exclude the effects of magnon-magnon interaction.

In this communication we focus on the study of configuration averaged dynamical response function of chemically disordered binary alloys. We shall use Augmented Space Recursion (ASR) technique proposed by one of us to study the environmental effects in chemically disordered alloys, taking it beyond the usual single site mean field coherent potential approximation (CPA) like approach. We have calculated the spin-spin correlations \( C(\vec{R}, \vec{R}', t, t') \) related to dynamical magnetic response of chemically disordered binary alloy \( \text{Fe}_x\text{Co}_{1-x} \). We propose a combination of the linear muffin-tin orbitals (LMTO) technique, augmented space formalism (AS)\textsuperscript{24},\textsuperscript{28, 34} and generalized recursion (GR)\textsuperscript{35, 38} to provide an accurate computational framework for analysing dynamical properties close to thermal equilibrium. We have also obtained the dynamical susceptibility \( \chi(\vec{q}, \omega) \gg \)\textsuperscript{39}, which determines the response of the system to a perturbation varying both in space and time, as well as the dynamical correlation functions \( C(\vec{q}, \omega) \gg \)\textsuperscript{36}, which relate the spontaneous fluctuations of the system to its response to an external perturbation.

\[
\ll \chi^+(\vec{q}, \omega) \gg = -\left( \frac{\mu_0 g \hbar^2}{V} \right) \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} d\vec{R} \ll C(\vec{R}, \tau) \gg \exp[-i(\vec{q} \cdot \vec{R} - \omega \tau)]
\]

where, \( \tau = t - t' \), \( \vec{R} = \vec{R} - \vec{R}' \)

\[
\ll C(\vec{R}, \tau) \gg = \ll \sigma^+(\vec{R}, t); \sigma^-(\vec{R}, t') \gg ; \text{is the spin-}
\]
correlation function and $-\frac{1}{2}$ Im $m \ll \Sigma(q, \omega) \gg 1/\tau_0$; all other symbols have their usual meanings. This implies the so called vertex corrections $\ll \Sigma(q, \omega) \gg$ in the Kubo type scattering formulated by us in the subsequent section. The singularities of the complex susceptibility constitute the magnon spectrum, leading to the dispersion relation: $\omega = \omega(q)$. Here $\ll \ldots \gg$ indicates a configurational averaged quantity in case of a disordered system, which is described by augmented space recursion technique discussed in detail in a subsequent section.

Because our system is chemically disordered, large scale inhomogeneities in the system ensure that $\chi^\pm(\vec{R}, \vec{R}', \omega) \neq \chi^\pm(\vec{R} - \vec{R}', \omega)$. Floquet-Bloch’s theorem is invalid and quantum states labelled by real reciprocal space vectors $\vec{q}$ have only finite lifetimes. However, if we describe the system in terms of configuration averages and if the probability densities are themselves lattice translationally invariant, we can return to the familiar homogeneous picture. The symmetry cannot be restored in the Hilbert space with a single random configuration of the Hamiltonian, but only if we have a formulation in which we work in the ‘augmented’ space of all possible random configurations. In fact, even if we have short ranged correlations, once such correlations themselves have translational symmetry, e.g. short-ranged order (SRO) parameter is the same at every site, the augmented space approach can be modified and has been done so. Only in extreme cases where the disorder itself (as characterized by the probability densities) is intrinsically inhomogeneous that the current approach begins to fail.

### A. Spin transport at low temperatures.

We analyse spin transport in ferromagnetic alloys. We begin with a ferromagnetic sea as our unperturbed state. A spin flip is an excitation or fluctuation in that state. We re-interpret the XXZ Heisenberg Hamiltonian with a random distribution of the exchange parameters $(J(\vec{R} - \vec{R}'))$ in terms of creation and annihilation operators of such fluctuations and their ‘transfer’ through the lattice:

$$H = -\sum_{\vec{R}} \sum_{\vec{R}'} J(\vec{R} - \vec{R}') \left( a^\dagger_{\vec{R}'} a_{\vec{R}} + a^\dagger_{\vec{R}} a_{\vec{R}'} + \Delta n_{\vec{R}} n_{\vec{R}'} \right)$$

(4)

where $\Delta$ is the anisotropic exchange parameter describing magnon-magnon interaction, $J(\vec{R} - \vec{R}')$ is the strength of the exchange interaction and $n_{\vec{R}} = a^\dagger_{\vec{R}} a_{\vec{R}}$. The excitations described in this model: spin waves or magnons can be envisaged as spin-patterns against a uniform spin background moving on the underlying lattice. The Hilbert space $H$ ($H \in \mathcal{H}$) is spanned by these “spin pattern” states. We begin with the model of ion cores sitting on the lattice immersed in a bonding sea of electron provided by atoms where they bond to form a solid.

![Figure 1](image)

Figure 1: (Color Online) (left panel) Ion cores immersed in a valence electron cloud which provides the bonding. (middle panel) Space divided into non-overlapping Weiner-Seitz cells with their own ion cores. (right panel) Wigner-Seitz cells replaced by sphere of the same volume. Now overlap must be less than 10%.

The use of the Heisenberg model has sometimes led to the misconception that we are dealing with discrete moments. A quick survey of the steps leading to the Heisenberg model will clarify this (Fig1). The model starts with ion cores immersed in an itinerant, bonding, valence electron clouds as shown in Fig1. Now we apply the DFT approach to obtain the Kohn-Sham equation:

$$\left[-\frac{1}{2} \nabla^2 + V_{eff}(\rho(r)r)\right] \Psi = e\Psi$$

(5)

We solve this equation by a real space muffin tin potentials model where initially we divided the space into Wigner-Szitz cells with its core at center as shown in Fig1. Then we replace the Wigner-Seitz cells by the corresponding inscribed spheres. The solution of the total energy from the Kohn-Sham methodology comes from the above model. We also obtain the total magnetization $M(\vec{R})$ within the atomic sphere so that: $M(\vec{R}) = \int_{AS} \rho^2 m(\vec{r})$. We should note this approach is based on an itinerant picture of bonding electron leading to magnetization densities rather than localised magnetic moment.

A first-principles determination of the pair-energy functions $J(\vec{R} - \vec{R}')$ requires careful consideration. This is a small energy difference of large energies:

$$J^{AB}(\vec{\chi}) = E^{A\uparrow,B\uparrow}(\vec{\chi}) + E^{A\downarrow,B\downarrow}(\vec{\chi}) - E^{A\uparrow,B\downarrow}(\vec{\chi}) - E^{A\downarrow,B\uparrow}(\vec{\chi})$$

Here $E^{A\sigma,B\sigma'}(\vec{\chi})$ is the total energy of a chemically disordered system where two sites $\vec{R}$ and $\vec{R}'$ are fixed with atoms of the type $A\sigma$ and $B\sigma'$, $\vec{\chi} = \vec{R} - \vec{R}'$. We can think of this as a perturbative problem and calculate the phase shift due to the immersion of $A$ and $B$ in the disordered background. Here we put disorder in the exchange terms to make the alloy chemically impure. The randomness can be introduced in the exchange parameter through a local, binary random variable $n_{\vec{R}} (\vec{R}$ can be occupied by $A$ or $B$ type of atom) taking the values 0 and 1 with probabilities $x$ and $y = 1 - x$:
leads to $<\phi_n|\phi_{n+1}> = 0 \Rightarrow \alpha_n = <\phi_n|H|\phi_n>

\beta_n = <\phi_{n+1}|\phi_{n+1}>

Substituting this in Eqn.(7), we get:

$$i\partial D_n(\vec{q},t)/\partial t = D_{n-1}(\vec{q},t) - \alpha_n D_n(\vec{q},t) - \beta_{n+1}^2 D_{n+1}(\vec{q},t)$$

Taking the Laplace Transformation:

$$(z - \alpha_n)\tilde{D}_n(\vec{q},z) - i\delta_{n0} = \tilde{D}_{n-1}(\vec{q},z) + \beta_{n+1}^2 \tilde{D}_{n+1}(\vec{q},z)$$

whence,

$$\tilde{D}_0(\vec{q},z) = \frac{i}{z - \alpha_1 - \beta_1^2 - \alpha_2 - \beta_2^2 - \alpha_3 - \ldots}$$

The structure function is then

$$C(\vec{q},\omega) = \lim_{\delta \to 0} \text{Re} \, e^{\delta}\tilde{D}_0(\vec{q},\omega + i\delta)$$

B. Recursive approach to dynamical spin response functions

Our starting point is a dynamical variable described by the Hermitian operator $D$, and our aim is to describe the time evolution of $|\Phi(t)\rangle = D(-t)|\Phi_0\rangle$. Our guiding equation is the Kohn-Sham equation:

$$\frac{\partial|\Phi(t)\rangle}{\partial t} = H|\Phi(t)\rangle$$

We shall follow the procedure described by Gagliano and Balseiro and Viswanathan and Muller. We first choose a denumerable basis of representation $\{|\phi_n\rangle\}$ and expand the “wave function” in this basis:

$$|\Phi(t)\rangle = \sum_{n=1}^{\infty} D_n(\vec{q},t)|\phi_n\rangle$$

We begin with $|\phi_1\rangle = \sigma^-(\vec{q})|\Phi_0\rangle$ where

$$\sigma^-(\vec{q}) = (1/N)^{1/2} \sum_{\vec{R}} e^{-i\vec{q}\cdot\vec{R}} \sigma^-(\vec{R})$$

Next step, $|\phi_2\rangle = H|\phi_1\rangle - \alpha_1|\phi_1\rangle$ and orthogonality leads to $<\phi_1|\phi_2> = 0 \Rightarrow \alpha_1 = <\phi_1|H|\phi_1> / <\phi_1|\phi_1>$. Finally for $n > 2$:

$$|\phi_{n+1}\rangle = H|\phi_n> - \alpha_n|\phi_n> - \beta_n^2 |n-1>$$

orthogonality $<\phi_n|\phi_{n+1}> = 0 \Rightarrow \alpha_n = <\phi_n|H|\phi_n>

\beta_n = <\phi_{n+1}|\phi_{n+1}>

C. Dynamical spin response functions in the presence of disorder : the augmented space approach

The linear response to an external homogeneous disturbance is discussed in terms of configuration averaged two particle Green’s functions and the Kubo-Greenwood approach. If a spin system is disturbed by an external field which causes a perturbation in XXZ Heisenberg Hamiltonian then in a homogeneously disordered system the spin response is related to this disturbance by a spin response function $\Gamma$:

$$\Gamma(\vec{R},\vec{R}',t-t') = \frac{i}{\hbar} \Theta(t-t') \langle \Phi_0|\sigma(\vec{R},t),\sigma(\vec{R}',t')|\Phi_0\rangle$$

$\sigma^\mu(\vec{R},t)$ is the spin operator, $\Theta$ is the Heaviside step function and $|\Phi_0\rangle$ the ground state.

$$\ll \Gamma(\vec{q},z) \gg = \langle \vec{q} \otimes \{\emptyset\}|(z\vec{I} - \vec{H})^{-1}|\vec{q} \otimes \{\emptyset\}\rangle$$

In the presence of disorder, $J(\vec{R} - \vec{R}')$ becomes a function of a set of random variables $\{n_{\vec{R}}\}$. The augmented space method replaces these variables $\{n_{\vec{R}}\}$ by operators $\{\lambda_{\vec{R},k}\}$ whose eigenvalues $\lambda_{\vec{R},k}$ are the random values taken by the variables and whose spectral functions are their probability densities. $J(\vec{R} - \vec{R}')$ is now an operator in the space of configurations. The augmented space theorem states that the matrix element between the “reference state” $\prod_{\vec{R}} \otimes \sum_{k} \sqrt{Pr(n_{\vec{R}} = \lambda_{\vec{R},k})}\phi(\lambda_{k})$ is the configuration average (see Ref. for details).
The configuration averaged response and spin correlation functions are:

\[
\langle \Gamma(q, z) \rangle = \langle q \otimes \{0\} | (zI - \hat{H})^{-1} | q \otimes \{0\} \rangle
\]

\[
\langle C(R - R', t - t') \rangle = \langle \{0\} | \hat{\sigma}(R, t) \hat{\sigma}(R', t') | \{0\} \rangle \quad (14)
\]

where \( z = \omega + i\delta \)

\[
\langle \hat{D}_0(q, z) \rangle = \frac{i}{\beta_2^2} \frac{z - \hat{\alpha}_1}{z - \hat{\alpha}_2 - \frac{\beta_2^2}{\beta_3^2} z - \alpha_3 \ldots}
\]  \quad (15)

The configuration averaged structure function is:

\[
\langle C(q, \omega) \rangle = \lim_{\delta \to 0} \text{Re} e \langle \hat{D}_0(q, \omega + i\delta) \rangle \quad (16)
\]

The fluctuation dissipation theorem relates the imaginary part of the Laplace transform of the generalized susceptibility (response) \( \langle \chi(q, \omega) \rangle \) to the Laplace transform of a correlation function \( \langle C(q, \omega) \rangle \) given by:

\[
\langle \chi(q, \omega) \rangle = (1/2\hbar) (1 - \exp(-\beta \hbar \omega)) \quad \langle C(q, \omega) \rangle \quad (17)
\]

The configuration averaged dynamical structure factor \( \langle C(q, \omega) \rangle \) is obtained, as before, through the recursive procedure suggested by Viswanath and Müller combined with Kubo-Greenwood formula. The self-energy \( \Sigma(q, z) \) via the recursion method suggested by Viswanath and Müller:

\[
\Sigma(q, z) = \frac{\beta_2^2}{z - \alpha_2} - \frac{\beta_3^2}{z - \alpha_3} - \ldots
\]  \quad (18)

where \( \{\alpha_n, \beta_n\} \) are Continued fraction recursion coefficients. Analyticity preserving approximations of continued fraction expansions has a rich literature based on terminators. The terminator \( T(q, z) \) is constructed out of the calculated \( \{\alpha_n, \beta_n\} \) \( n = 1, \ldots, N \) and reflects all the singularities of the exact response functions. This method requires no external parameters to be introduced and the smoothing automatically comes from the terminator. This \( \text{Im} m(S(q, \omega)) = 1/\tau_0 \) is the disorder induced lifetime of a \( q \) labeled quantum state. The structure function \( C(q, \omega) \), which is the Laplace transform of the correlation function \( C(R, t - t') \) can then be obtained from in Eqn.(16). Thus two particle dynamical spin response function is given by:

\[
\langle \Gamma(q, t) \rangle = -i e^{-i(E_0(q) + \Delta E)t/\gamma_0} \quad (19)
\]

We have chosen disordered binary alloy Fe\(_x\)Co\(_{1-x}\) for varying concentrations of \( x \). We use the \( q \)-space algorithm over mean-field and super-cell approaches because we did not wish to introduce artificial periodicity and miss out on the effects of long-ranged disorder. The problem with any numerical calculation is that we can deal with only a finite number of computation operations. In the recursion algorithm, we can go up to a finite number of steps and if we stop the recursion, this would lead to exactly what we wish to avoid. The analysis of the asymptotic part of the continued fraction is therefore of prime interest to us. This is the “termination” procedure discussed by Haydock and Nex, Luchini and Nex, Beer and Pettifor and in considerable detail by Viswanath and Müller. This terminator \( T(z) \) which accurately describes the far environment, must maintain the herglotz analytical properties. We have to incorporate not only the singularities at the band edges, but also those lying on the compact spectrum of \( \hat{H} \) or in the gaps. We calculate the continued fraction recursion coefficients \( (\beta_n) \) for a \( d \)-projected structure function for thirty recursion steps that we able to go. The coefficients \( (\beta_n) \) do show a tendency for oscillatory convergence. The parameters of the terminator are estimated from the asymptotic part of the continued fraction coefficients calculated from our recursion. We therefore choose square-root terminator coefficients seamlessly enmeshed with the calculated recursion coefficients \( (\beta_n) \). In this way both the near and the far environments are accurately taken into account. We use the Cambridge Recursion Library to accurately locate the band edges and hence constructed the necessary terminator for each angular momentum projected continued fraction (spectral density or correlation function).

### D. Atomistic spin dynamics and numerical details

We calculated the magnon dispersion relation of Fe\(_x\)Co\(_{1-x}\) \((x=0.8, 0.5\) and 0.2\) alloys using UppASD (Uppsala Atomistic Spin Dynamics) code. The UppASD code is based on the framework of LLG formalism. The temporal evolution of an atomic moment in LLG formalism is given by:

\[
\frac{d\mathbf{m}_i(t)}{dt} = -\frac{\gamma}{1 + \alpha^2} \mathbf{m}_i(t) \times [\mathbf{H}_i^{\text{eff}} + \alpha \frac{m_s}{m} (\mathbf{m}_i(t) \times \mathbf{H}_i^{\text{eff}})]
\]  \quad (20)

where \( \mathbf{m}_i(t) \) is the atomic moment on the \( i^{th} \) site at time \( t \). \( \gamma \) is the gyromagnetic ratio and \( \alpha \) is the Gilbert damping factor, which we have assumed to be 0.000303. \( m_s \) is the saturation moment for the \( i^{th} \) atom. The effective field \( \mathbf{H}_i^{\text{eff}} \) on the \( i^{th} \) atom is calculated from the effective magnetic Hamiltonian given by:

\[
\mathcal{H}_{Mag} = \mathcal{H}_{ex}
\]  \quad (21)
\[ \mathcal{H}_{\text{eff}}^i = - \frac{\partial \mathcal{H}_{\text{Mag}}}{\partial \mathbf{m}_i(t)}. \]

\( \mathcal{H}_{\text{ex}} \) describes the magnetic exchange interactions between the spins. \( \mathcal{H}_{\text{Mag}} \) is given by

\[ \mathcal{H}_{\text{Mag}} = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \]

The necessary exchange parameters for ASD are calculated in the the framework of \textit{ab-initio} density functional theory (DFT). They were done by means of the Korringa-Kohn-Rostocker Green’s function formalism as implemented in the SPRKKR package\textsuperscript{51}. The shape of the potential was treated by the Atomic Sphere Approximation (ASA), while the relativistic effects were considered by taking the fully relativistic Dirac equation. The effect of the exchange correlation part of the energy was treated by considering the Generalized Gradient Approximation (GGA). The interatomic exchange interactions were calculated via the LKAG formalism.\textsuperscript{92}

In order to calculate magnon dispersion relation, one should calculate spin-spin correlation function. The spin-spin correlation in an effective field is obtained by solving the LLG equation and can be written as,

\[ C^k(\mathbf{r} - \mathbf{r}^\prime) = \langle m_r^k(t) m_{r^\prime}^k(0) \rangle - \langle m_r^k(t) \rangle \langle m_{r^\prime}^k(0) \rangle \] (22)

where the ensemble average is represented in the angular brackets and \( k \) is the cartesian component. The Fourier transform of the spin-spin correlation function, known as dynamical structure factor is written as,

\[ S(k,\omega) = \frac{1}{\sqrt{2\pi N}} \sum_{\mathbf{r},\mathbf{r}'} \int_{-\infty}^{\infty} e^{i\omega t} C^k(\mathbf{r} - \mathbf{r}^\prime, t) dt, \] (23)

\( S(\mathbf{q}, \omega) \) is measured in neutron scattering experiments.

### III. RESULTS AND DISCUSSION

#### A. Spectral properties of valence electrons in ordered FeCo alloy

Before we proceed to formulate the TB-LMTO-ASR on response functions, let us first apply the technique to study spectral functions of the valence electrons of body-centered disordered 50-50 FeCo alloy. Fig. 2 compares the PDOS of the disordered with the corresponding ordered B2 structured alloys. In all three alloys, the distinguishable features in the PDOS arises out of the underlying lattice geometry remains unchanged. What changes is the local chemical environments of the components. So the strongly distinguishable features of the PDOS is still seen in the disordered alloys. However, the sharp features and Van Hove singularities which characterize the ordered alloys are all smoothened out by life-time effects due to disorder driven fluctuations.

In Table I, we show the chemical effects of disorder and the redistribution of charge on alloying. The first thing we note that if we measure the ‘size’ of the atom by the atomic radius \( R_0 \) (muffin-tin radius) in the sense that we consider all the electronic cloud contained within this sphere as ‘belonging’ to the ion-core at its center, then in all three alloys the components have roughly the same radius. This has an important effect on the modeling of disorder within the LMTO. The off-diagonal terms in the Hamiltonian were:

\[ H_{\mathbf{R},L;\mathbf{R}',L'} = \Delta_{\mathbf{R},L}^{1/2} C(\mathbf{R}, L; \mathbf{R}', L') \Delta_{\mathbf{R}',L'}^{1/2} \] (24)

We had taken disorder in the potential parameters \( \Delta_{\mathbf{R},L}^{1/2} \) which are local and chemistry driven, but neglected any disorder in the structure matrix.
\( C(\tilde{R}, L, \tilde{R}', L') \) which depends on the underlying lattice structure alone. If, however, the atomic ‘sizes’ of the components are very different (as in CuBe or beryllium bronze) then we have to replace the average structure matrix by:

\[
S^{AA}(\tilde{R}, L; \tilde{R}', L') n_{\tilde{R}A} n_{\tilde{R}'} + S^{BB}(\tilde{R}, L; \tilde{R}', L') (1 - n_{\tilde{R}})(1 - n_{\tilde{R}'}) \\
\ldots + S^{AB}(\tilde{R}, L; \tilde{R}', L') \{ n_{\tilde{R}}(1 - n_{\tilde{R}'}) + (1 - n_{\tilde{R}})n_{\tilde{R}'}) \}
\]

This would lead to local lattice distortion wherever a large or small atom sits. Our ASR technique can very easily take this into account without any modification and has been used earlier to study CuBe alloys\(^{27}\).

In these alloy, there is a small decrease of sp like charges and a corresponding small increase in the d like channel in Fe, with the effect being increased with the introduction of disorder. This charge transfer effect is almost negligible for FeCo.

### B. Dynamical response function

The augmented space recursive approach has been applied to study the magnetization dynamics in disordered ferromagnetic body-centered cubic, transition metallic Fe\(_x\)Co\(_{1-x}\) alloys. The calculated magnon softening for Fe\(_{20}\)Co\(_{80}\) at \( T = 0 \) K is found to be in very good agreement with the results based on the scattering theory approach. Ebert et al. have tried to include disorder through the coherent potential approximation (CPA)\(^{12}\). The results are inadequate. This led them to use the non-local CPA, which is an analyticity preserving extension of the CPA\(^{58}\). We have used the augmented space recursion (ASR) method. Both the CPA and NLCPA are special cases derivable from the AST\(^{59,61}\). An indispensable requirement to achieving this agreement is to include the vertex corrections mentioned above. In fact, ignoring them leads in some cases to completely unphysical results. While the scattering and linear response approach are completely equivalent when dealing with bulk alloys, the latter allows us to perform the necessary configuration averaging in disordered alloy in a much more efficient way. This allows us to study with moderate effort the influence of varying the alloy composition on the magnon softening of Fe\(_x\)Co\(_{1-x}\) alloy. Furthermore, the obtained strong damping of short wave vector magnons in Fe\(_x\)Co\(_{1-x}\) compounds suggests a q-dependent damping constant \( a_q \) in the LLG equation in describing magnetization dynamics of large-angle fast precessional switching\(^{12}\). Interaction of itinerant ferromagnets with single-particle Stoner excitation is neglected here as it is usually present for large wave vector (q) magnon. We confine ourselves in linear spin wave regime (LSWT) of short wave vector (q) magnon. Since we take the bulk ferromagnets of cubic symmetry, so we have neglected the magnetic anisotropic contribution.

We only take chemical disorder in our consideration. We may compare our results with those of Anders Bergman et al.\(^{14}\) on Fe/W(110) monolayer system based on similar approaches. We have to note though that their calculation involved actual dynamics of moment relaxation based on adiabatic approximation, while ours was an equilibrium approach.

The ensemble averaged dynamical structure function \( \ll C(q, \omega) \gg \) can easily be obtained from neutron scattering\(^{62}\) and spin-polarized electron energy loss spectroscopy (SPEELS)\(^{15}\) experiments. We should note here that as long as we are using configurationally averaged quantities and disorder is homogeneous, we can use reciprocal space, but with the proviso that the real energy spectrum is no longer labeled by \( q \) and the dispersion bands are no longer sharp. We have obtained the magnon dispersions by identifying the peak positions of the dynamical structure factor \( \ll C(q, \omega) \gg \) along particular directions in reciprocal space of disordered BCC alloy. After configuration averaging, in order to simplify the identification of the intensity peaks of dynamical structure factor \( \ll C(q, \omega) \gg \) the intensity for each \( q \) vector is convoluted with a Lorentzian function, normalized to unity. The \( q \)-dependent dynamical structure function \( C(q, \omega) \) is a central quantity for the understanding of magnetism. Fig.3 shows the dynamical structure function \( \ll C(q, \omega) \gg \) convoluted with a Lorentzian function for the disordered binary body centered cubic Fe\(_x\)Co\(_{1-x}\) alloy for three concentrations of x (disorder) with x=0.2, 0.5, 0.8 respectively. The figure displays the calculated dynamical structure factors, for a selection of different \( q \) vectors varying from 0.0 to 0.9 along the symmetric \( \Gamma - Y \) direction i.e. [001] in the reciprocal space of BCC lattice. For low \( q \) values, the spectral intensity of is high, and decreases with increasing \( q \). At the same time, the peak width can be seen to increase with increasing energy as well as wave vector (q). This is made clear by observing the peaks located at \( q = 0.1 \) \( \text{Å}^{-1} \) and 0.8 \( \text{Å}^{-1} \) of three alloy compositions. The broadening of higher energy excitations can be explained by the stronger disorder induced scattering at large \( q \) i.e. smaller modes. As stated earlier we neglect the effect of spin wave (magnon-magnon) interaction and Stoner excitation. Stoner continuum in bulk systems is quite different as compared with low dimensional systems and usually present for large wave vector (q) magnons. Here we mainly deal with short wave vector magnons. As there is no dynamical correlation due to the absence of magnon-magnon interactions, broadening of peak in dynamical structure factors \( C(q, \omega) \) comes from magnon-electron scattering mechanism due to chemical impurity. The itinerant collective excitations (spin waves) lose their magnon energy due to chemical disorder induced spin-flip transitions between occupied majority (spin-up) and unoccupied minority (spin-down) states. This magnon energy loss reduces its lifetime drastically which leads to magnon softening of Fe\(_{0.2}\)Co\(_{0.8}\) alloy. A large damping of magnons in the tetragonally distorted bulk FeCo com-
pounds is also predicted previously\textsuperscript{63, 64}.

Figure 3: (Color Online) The dynamical structure factors $S(\vec{q}, \omega)$ for a selection of wave vectors $\vec{q}$ varying from 0.0 to 0.9 along the symmetric $\Gamma - Y$ direction i.e. [001] in the reciprocal space of BCC Fe\textsubscript{1-x}Co\textsubscript{x} alloys (top) $x=0.2$ (middle) $x=0.5$ (bottom) $x=0.8$ respectively. In order to identify the peak position the dynamical structure function $\ll S(\vec{q}, \omega) \gg$ are convoluted with a Lorentzian function, normalized to unity. Magnon softening is observed for Fe\textsubscript{0.2}Co\textsubscript{0.8} alloy at higher $\vec{q}$ values. For low wave vectors $q$, the spectral peaks are strongly intense. The spectral peak width can be seen to increase with increasing energy as well as wave vector ($q$). This leads to more magnon damping at higher $\vec{q}$ values at all concentration.

Table II: Exchange parameters

| Alloy    | $Fe - Fe$ | $Fe - Co$ | $Co - Co$ |
|----------|-----------|-----------|-----------|
| Fe\textsubscript{50}Co\textsubscript{0} | 2.065     | 2.302     | 1.740     |
| Fe\textsubscript{50}Co\textsubscript{0.2} | 2.083     | 2.117     | 1.418     |
| Fe\textsubscript{50}Co\textsubscript{0.8} | 1.919     | 1.880     | 1.208     |

Table III: Magnetic moments

| Alloy    | $Fe$ $\mu_B$ | $Co$ $\mu_B$ | Total $\mu_B$ |
|----------|---------------|---------------|---------------|
| Fe\textsubscript{50}Co\textsubscript{0} | 2.50          | 1.78          | 4.28          |
| Fe\textsubscript{50}Co\textsubscript{0.2} | 2.59          | 1.76          | 4.36          |
| Fe\textsubscript{50}Co\textsubscript{0.8} | 2.62          | 1.73          | 4.35          |

The disagreement. The experiments have been done on a chemically disorder alloy is not the main reason for the disagreement. 

As the concentration of Co increases, the calculated magnon spectrum for Fe\textsubscript{50}Co\textsubscript{x} alloys more explicitly with experimental data of Qin et.al on bulk ferromagnetic BCC Fe (ordered)\textsuperscript{65}. Mook et.al experimentally reported previously that BCC ordered Bulk Fe system has a spin-wave stiffness constant of 280 meV $\text{Å}^2$ displayed in Fig.4\textsuperscript{68} also. We find the quadratic dependence upon $\vec{q}$ for the spin wave spectrum of a magnon in the itinerant Heisenberg model of disordered Fe\textsubscript{1-x}Co\textsubscript{x} alloy. Fe\textsubscript{80}Co\textsubscript{20} and Bulk Fe have almost similar nature of magnon spectrum. Now the magnon spectrum is gradually soften down if we increase Co content. The calculated magnon spectrum for Fe\textsubscript{50}Co\textsubscript{50} is displayed in Fig.4, together with the experimental data of Qin et.al\textsuperscript{69} for ultrathin ferromagnetic Fe\textsubscript{50}Co\textsubscript{50} films grown on Ir(001), and the experimentally determined spectrum for bulk bcc Fe\textsuperscript{68} by Mook et.al. The agreement with the SPEELS data on ferromagnetic film of disordered Fe\textsubscript{50}Co\textsubscript{50} is quite well, particularly for low wave vector region and magnon softening is captured at the zone boundary. Ultrathin ferromagnetic Fe\textsubscript{50}Co\textsubscript{50} films have a large perpendicular magnetic anisotropy due to tetragonal distortion. At low wave vectors both bulk and ultrathin ferromagnetic Fe\textsubscript{2}Co\textsubscript{1-x} films possess almost identical magnon energies. But chemical disorder leads to strong magnon softening at the zone boundary for bulk Fe\textsubscript{50}Co\textsubscript{50} in comparison with ultrathin ferromagnetic films here. The disagreement between our theoretical estimation, which includes disorder and experiment of Qin et.al\textsuperscript{69} leads us to doubt the statement of Qin et.al. The inter-mixing of Fe and Co resulting in a chemically disorder alloy is not the main reason for the disagreement. The experiments have been done on ultrathin films grown on Ir(001) substrate while our calculations are in the bulk. Similar to the work of Anders et.al\textsuperscript{14} we observe the strong softening of the $\vec{q}$ labelled modes at zone boundary for the Fe\textsubscript{80}Co\textsubscript{20} alloy which indicates a strong reduction of the Curie temperature in Fe\textsubscript{20}Co\textsubscript{80} alloy\textsuperscript{63}.

Ebert et.al calculated Gilbert damping parameter $\alpha$ from first principles theory for bcc disordered Fe\textsubscript{1-x}Co\textsubscript{x} alloys\textsuperscript{12}. Damping is minimum for 20% Co content and gradually increases with adding Co content. This leads to strong magnon softening in Fe\textsubscript{20}Co\textsubscript{80} alloy. Our result is also consistent with experiment done by Oogane et.al on bcc Fe\textsubscript{1-x}Co\textsubscript{x} alloy\textsuperscript{70}. This strong magnon softening is in contradiction with previous study based on an itinerant electron model at $T = 0$ K\textsuperscript{71, 72} and revealed the possibility that a disordered Fe\textsubscript{1-x}Co\textsubscript{x} may not be a simple itinerant ferromagnet in low temperature, the effects of spin correlations are important for that system. This behavior is commonly interpreted as a transition from conductivity like to resistivity like behavior reflecting the dominance of intra and interband transition, respectively, that is related to the increase of the broadening of electron energy bands caused by the increase of scattering events with...
Figure 4: (Color Online) Magnon dispersion spectra for bulk, ferromagnetic and disordered binary (top) Fe$_{20}$Co$_{80}$, (middle) Fe$_{50}$Co$_{50}$ and (bottom) Fe$_{80}$Co$_{20}$ alloys respectively along the symmetric Γ−Y direction i.e. [001]. We compare our data with the experimental spin-wave spectrum of bulk bcc Fe (corresponding to a spin-wave stiffness constant of 280 meV Å$^2$) by Mook et al.\cite{68}.

A further increase of the Co content leads to the impurity-scattering processes responsible for band broadening dominating damping. This effect completely suppresses the conductivity like behavior in the low temperature regime because of the increase of scattering due to chemical disorder. In the absence of spin orbit coupling (SOC) the angular momentum stays in the magnetic subsystem, i.e., it is transferred from magnons to the non-coherent single-particle spin-flip itinerant excitations. The SOC is responsible for angular momentum transfer from the magnetic subsystem to the lattice subsystem. We also note that we have not included SOC in the calculation of the dynamical response function. Ab-initio calculations by Lezaic et al.\cite{73} and Jakobsson et al.\cite{64} on cubic ordered and disordered Fe$_x$Co$_{1-x}$ alloys agrees well with our views. The large magnon softening suggests Fe$_x$Co$_{1-x}$ to be a promising material for recording applications. Literature survey shows a lack of direct available experimental data for disordered Fe$_{20}$Co$_{80}$ alloy, but implicitly magnon softening in disordered Fe$_{20}$Co$_{80}$ is confirmed by experiments\cite{74-77}.

The broadening of the magnon excitation peak ($S(\vec{q},\omega)$) provides a way of estimating the magnon lifetime $\tau_0$. We obtain disorder induced lifetime $\tau_0$ of a $\vec{q}$ labeled quantum state from the self-energy for these alloys. Fig. 5 shows the variation of lifetime $\tau_0$ as a function of $\vec{q}$ (Å$^{-1}$) together with the experimental data of Qin et al.\cite{69} for Fe$_{50}$Co$_{50}$ alloy. The relaxing magnetic modes or patterns are labelled by $\vec{q}$, such that the average ‘size’ of the mode is $O(q^{-1})$. We note that magnon lifetime decreases with its wave vector. Due to strong damping, terahertz magnons possess a very short lifetime being in the order of a few tens of femtoseconds\cite{20,21}.

We shall now compare our work with an earlier experimental and theoretical study of very similar systems. We shall begin with the experimental report by Zhang et al.\cite{20} on the relaxation of terrahertz magnons. The results were obtained by using spin-polarized electron energy loss spectroscopy (SPEELS)\cite{15}. The choice of the experimental technique was guided by the fact that SPEELS can access both the energy and wave function of large wave-vector magnons\cite{78-81}. The energy $E(\vec{q})$ and its spread is extracted from the raw difference spectra data by fitting them to a convolution of Gaussian (describing the instrumental broadening) and a Lorentzian (describing intrinsic disorder induced broadening). The authors quote that the latter dominates the broadening, specially for megahertz magnons. This is consistent with our model, where we have neglected the instrumental broadening altogether. The large broadening of the loss spectrum indicates that magnons are strongly damped in
Figure 6: The upper row figures ((a)-(c)) show the magnon dispersion of Fe$_x$Co$_{1-x}$ (where $x = 0.8, 0.5$ and $0.2$) alloys with nearest neighbor exchange parameters and the lower row has the plots ((d)-(f)) with 12 neighbour shells’ exchange parameters.
time. We have obtained the magnon lifetimes from the Fourier transform of the configuration averaged correlation function. The Fourier transform of the Lorentzian in energy (or frequency) domain is an exponential decay function. The Fourier transform of the Lorentzian Fourier transform of the configuration averaged correlation time. We have obtained the magnon lifetimes from the different in ASR and ASD simulations.

The ASD simulations are performed with a system size of 120x120x120 at a temperature of 0.1K. The calculated dynamical structure factors or the energy spectra $S(q, \omega)$ of FeCo alloys are shown in Fig.6 along the high symmetry directions in the Brillouin zone. In the upper panel we show magnon dispersion relations calculated using nearest neighbor (nn) exchange interaction only and in the lower panel, the results of 12 neighbor exchange interactions are shown. The qualitative features in the magnon spectra for nn and 12 neighbor shells are similar but some quantitative differences are visible. Specifically, a stronger tendency for branching is visible at the N point of the Brillouin zone with 12 neighbor interactions. The broadening of magnon spectra is similar to that obtained from ASR calculations shown above. However, it should be noted that the magnon energies are quantitatively different in ASR and ASD simulations.

IV. CONCLUSION

In conclusion, here we have focused on the development of combining first-principles TB-LMTO calculations with ASR-Kubo-Greenwood as a general computational technique provides a powerful tool for studies of the effect of disorder on magnetic excitations in bulk as well as in low-dimensional systems. There are other competing mechanisms which we have to build into our model if we want a more realistic picture. Most importantly, spin-orbit coupling leading to a Dzyaloshinskii-Moriya term in the Hamiltonian will couple magnons with the lattice and phonon-magnon scattering will play an important role. The relativistic version of augmented space recursion is already available with us to undertake this extension. Unlike some earlier work, the way we have estimated the pair energy through space-orbital peeling, the chemical effect of alloying Fe with Co is implicitly included in our work. We apply our technique to study the magnetization dynamics of disordered binary Fe$_x$Co$_{1-x}$ alloys which are of great fundamental as well as technological interest. The method captures a significant magnon softening of Fe$_{20}$Co$_{80}$ compared to bulk Fe. These results are supported by our atomistic spin dynamics simulations with the exchange parameters calculated from ab-initio theory. Our suggestion is further exploration of this technique to calculate the spin conductivity of Heisenberg chains in alloys.

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1. I. Tudosa, C. Stamm, A. B. Kashuba, F. King, H. C. Siegmann, J. Störh, G. Ju, B. Lu, and D. Weller, Nature London 428, 831 (2004).
2. G. D. Fuchs, N. C. Emley, I. N. Krivorotov, P. M. Braganca, E. M. Ryan, S. I. Kiselev, J. C. Sankey, D. C. Ralph, R. A. Buhrman and J. A. Katine, Appl. Phys. Lett. 85, 1205 (2004)
3. J. C. Sankey, Y.-T. Cui, J. Z. Sun, J. C. Slonczewski, R. A. Buhrman and D. C. Ralph, Nat. Phys. 4, 67 (2008).
4. B. Heinrich and J.F. Cochran, Adv. Phys. 42, 523 (1996)
5. H. Kubota et.al., Nat. Phys. 4, 37 (2008).
6. L. Berger, Phys. Rev B54 9353 (1996)
7. J.C. Sionczewskii, J. Magn. Magn. Mater. 159 L1 (1996)
8. Vladimir L. Safovon and H. Neal Bertram Journal of Applied Physics 93, 6912 (2003); DOI: 10.1063/1.1543891
9. Vladimir L. Safovon Journal of Applied Physics 85, 4370 (1999); DOI: 10.1063/1.369787
10. Vladimir L. Safovon Journal of Applied Physics 95, 7145 (2004); DOI: 10.1063/1.1688681
11. Vladimir L. Safovon and H. Neal Bertram Journal of Applied Physics 94, 529 (2003); DOI: 10.1063/1.1581349
12. H. Ebert, S. Mankovsky, and D. Kodderitzsch PRL 107, 066603 (2011)
13. B. Skubic, J. Hellsvik, L. Nordström, and O. Eriksson, J. Phys. Condens. Matter
14. Anders Bergman, Andrea Taroni, Lars Bergqvist, Johan Hellsvik, Björgvin Hjörvarsson, and Olle Eriksson Phys. Rev. B 81, 144416 (2010) DOI: 10.1103/PhysRevB.81.144416 20, 315203 2008.http://www.fysik.uu.se CMT/ASD
15. S. Dalosto and J. Riera Phys. Rev. B 62, 928 (2000)
16. H. Hopster, Spin-polarized electron energy loss spectroscopy, Surf. Rev. Lett. 01 (01), (1994) 89-96.
17. R. Vollmer, M. Etzkorn, P.S.A. Kumar, H. Ibach, J. Kirschner, Spin-polarized electron energy loss spectroscopy of high energy, large wave vector spin waves in ultrathin fcc co films on cu(001), Phys. Rev. Lett. 91, (2003) 147201.
18. R. Vollmer, M. Etzkorn, P. Kumar, H. Ibach, J. Kirschner, Spin-wave excitation observed by spin-polarized electron energy loss spectroscopy: a new method for the investigation of surface- and thin-film spin waves on the atomic scale, Thin Solid Films 464 - 465, (2004) 42-47.
19. R. Vollmer, M. Etzkorn, P.A. Kumar, H. Ibach, J. Kirschner, Spin-polarized electron energy loss spectroscopy: a method to measure magnon energies, J. Magn. Magn. Mater. 272–276, (2004) 2126–2130.
20. Y. Zhang, T.-H. Chuang, Kh.Zakeri and J.Kirschner . Phys. Rev. Lett. 109, 087203 (2012) DOI: 10.1103/PhysRevLett.109.087203
21. K. Zakeri, Y. Zhang, T.-H. Chuang, and J. Kirschner, Phys. Rev. Lett. 108, 197205 (2012).
22. V.P. Antropov, M. I. Katsnelson, B. N. Harmon, M. van Schilfgaarde, and D. Kusnezov, Phys. Rev. B 54, 1019 (1996).
L. Liu, O. J. Lee, T. J. Gudmundsen, D. C. Ralph, and R. A. Buhrman, \textit{Phys. Rev. Lett.} \textbf{109}, 096602 (2012).

http://physics.uu.se/forskning/materialteori/pagaende-forskning/uppasd/

V. P. Antropov, M. I. Katsnelson, B. N. Harmon, M. van Schilfgaarde and D. Kusnezov, \textit{Phys. Rev. B} \textbf{54}, 1019 (1996).

B. Skubic, J. Hellsvik, L. Nordström, O. Eriksson, Journal of Physics Condensed Matter, \textbf{20} 315203 (2008).

The Munich SPR-KKR package, version 6.3, H. Ebert \textit{et al}, http://ebert.cup.uni-muenchen.de/SPRKKR; H. Ebert, D. Ködderitzsch and J. Minár, Rep. Prog. Phys. \textbf{74}, 096501 (2011).

A. I. Liechtenstein, M. I. Katsnelson, and V. A. Gubanov, J. Phys. F: Met. Phys. \textbf{14}, L125 (1984); A. I. Lichtenstein, M. I. Katsnelson, V. P. Antropov, and V. A. Gubanov, J. Magn. Magn. Mater. \textbf{67}, 65 (1987).