Calculating linear response functions for finite temperatures on the basis of the alloy analogy model

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A scheme is presented that is based on the alloy analogy model and allows for thermal lattice vibrations as well as spin fluctuations when calculating response quantities in solids. Various models to deal with spin fluctuations are discussed concerning their impact on the resulting temperature dependent magnetic moment, longitudinal conductivity and Gilbert damping parameter. It is demonstrated that using the Monte Carlo (MC) spin configuration as an input, the alloy analogy model is capable to reproduce results of MC simulations on the average magnetic moment within all spin fluctuation models under discussion. On the other hand, response quantities are much more sensitive to the spin fluctuation model. Separate calculations accounting for either the thermal effect due to lattice vibrations or spin fluctuations show their comparable contributions to the electrical conductivity and Gilbert damping. However, comparison to results accounting for both thermal effects demonstrate violation of Matthiessen’s rule, showing the non-additive effect of lattice vibrations and spin fluctuations. The results obtained for bcc Fe and fcc Ni are compared with the experimental data, showing rather good agreement for the temperature dependent electrical conductivity and Gilbert damping parameter.

I. INTRODUCTION

Finite temperature has often a very crucial influence on the response properties of a solid. A prominent example for this is the electrical resistivity of perfect non-magnetic metals and ordered compounds that only take a non-zero value with a characteristic temperature \( T \) dependence due to thermal lattice vibrations. While the Holstein transport equation\(^{1,2}\) provides a sound basis for corresponding calculations numerical work in this field has been done so far either on a model level or for simplified situations.\(^{3–6}\) In practice often the Boltzmann-formalism is adopted using the constant relaxation time \( (\tau) \) approximation. This is a very popular approach in particular when dealing with the Seebeck effect, as in this case \( \tau \) drops out.\(^{7,8}\) The constant relaxation time approximation has also been used extensively when dealing with the Gilbert damping parameter \( \alpha \).\(^{9–11}\) Within the description of Kambersky\(^{10,12}\) the conductivity- and resistivity-like intra- and inter-band contributions to \( \alpha \) show a different dependency on \( \tau \) leading typically to a minimum for \( \alpha(\tau) \) or equivalently for \( \alpha(T) \).\(^{10,11}\) A scheme to deal with the temperature dependent resistivity that is formally much more satisfying than the constant relaxation time approximation is achieved by combining the Boltzmann-formalism with a detailed calculation of the phonon properties. As was shown by various authors,\(^{13–16}\) this parameter-free approach leads for non-magnetic metals in general to a very good agreement with experimental data.

As an alternative to this approach, thermal lattice vibrations have also been accounted for within various studies by quasi-static lattice displacements leading to thermally induced structural disorder in the system. This point of view provides the basis for the use of the alloy analogy, i.e. for the use of techniques to deal with substitutional chemical disorder also when dealing with temperature dependent quasi-static random lattice displacements. An example for this are investigations on the temperature dependence of the resistivity and the Gilbert parameter \( \alpha \) based on the scattering matrix approach applied to layered systems.\(^{17}\) The necessary average over many configurations of lattice displacements was taken by means of the super cell technique. In contrast to this the configurational average was determined using the Coherent Potential Approximation (CPA) within investigations using a Kubo-Greenwood-like linear expression for \( \alpha \).\(^{18}\) The same approach to deal with the lattice displacements was also used recently within calculations of angle-resolved photo emission spectra (ARPES) on the basis of the one-step model of photo emission.\(^{19}\)

Another important contribution to the resistivity in the case of magnetically ordered solids are thermally induced spin fluctuations.\(^{20}\) Again, the alloy analogy has been exploited extensively in the past when dealing with the impact of spin fluctuations on various response quantities. Representing a frozen spin configuration by means of super cell calculations has been applied for calculations of the Gilbert parameter for \( \alpha \)\(^{21}\) as well as the resistivity or conductivity, respectively.\(^{17,21,22}\) Also, the CPA has been used for calculations of \( \alpha \)\(^{23}\) as well as the resistivity.\(^{20,24}\) A crucial point in this context is obviously the modeling of the temperature dependent spin configurations. Concerning this, rather simple models have been used,\(^{25}\) but also quite sophisticated schemes. Here one should mention the transfer of data from Monte Carlo simulations based on exchange parameters calculated in an ab-initio way\(^{25}\) as well as work based on the disordered local moment (DLM) method.\(^{23,26}\) Although, the standard DLM does not account for transversal spin components it nevertheless allows to represent the paramagnetic regime with net magnetization in a rigor-
ous way. Also, for the magnetically ordered regime below the Curie-temperature it could be demonstrated that the uncompensated DLM (udDLM) leads for many situations still to good agreement with experimental data on the so-called spin disorder contribution to the resistivity.\textsuperscript{20,24}

In the following we present technical details and extensions of a scheme that was already used before when dealing with the temperature dependence of response quantities on the basis of Kubo’s response formalism. Various applications will be presented for the conductivity and Gilbert damping parameter accounting simultaneously for various types of disorder.

II. THEORETICAL FRAMEWORK

A. Configurational average for linear response functions

Many important quantities in spintronics can be formulated by making use of linear response formalism. Important examples for this are the electrical conductivity,\textsuperscript{27,28} the spin conductivity,\textsuperscript{29} or the Gilbert damping parameter.\textsuperscript{18} Restricting here for the sake of brevity to the symmetric part of the corresponding response tensor $\chi_{\mu\nu}$ this can be expressed by a correlation function of the form:

$$\chi_{\mu\nu} \propto \text{Tr} \left\langle \hat{A}_{\mu} \Sigma G^+ \hat{A}_{\nu} \Sigma G^+ \right\rangle_c .$$

It should be stressed that this not a real restriction as the scheme described below has been used successfully when dealing with the impact of finite temperatures on the anomalous Hall conductivity of Ni.\textsuperscript{31} In this case the more complex Kubo-Stˇreda- or Kubo-Bastin formulation for the full response tensor has to be used.\textsuperscript{12}

The vector operator $\hat{A}_{\mu}$ in Eq. (1) stands for example in case of the electrical conductivity $\sigma_{\mu\nu}$ for the current density operator $j_{\mu}$\textsuperscript{28} while in case of the Gilbert damping parameter $\alpha_{\mu\nu}$ it stands for the torque operator $T_{\mu\nu}$.\textsuperscript{3,9,18} Within the Kubo-Greenwood-like equation (1) the electronic structure of the investigated system is represented in terms of its retarded Green function $G^+(\mathbf{r}, \mathbf{r}', E)$. Within multiple scattering theory or the KKR (Korringa-Kohn-Rostoker) formalism, $G^+(\mathbf{r}, \mathbf{r}', E)$ can be written as:\textsuperscript{33-35}

$$G^+(\mathbf{r}, \mathbf{r}', E) = \sum_{\Lambda\Lambda'} Z^{m}_{\Lambda} (\mathbf{r}, E) \tau^{mn}_{\Lambda\Lambda'} (E) Z^{n}_{\Lambda'} (\mathbf{r}', E)$$

$$- \delta_{mn} \sum_{\Lambda} Z^{n}_{\Lambda} (\mathbf{r}, E) J^{mn}_{\Lambda} (\mathbf{r}', E) \Theta(r'_n - r_n)$$

$$+ J^{n}_{\Lambda} (\mathbf{r}, E) Z^{n}_{\Lambda} (\mathbf{r}', E) \Theta(r_n - r'_n) .$$

Here $\mathbf{r}, \mathbf{r}'$ refer to points within atomic volumes around sites $\mathbf{R}_m, \mathbf{R}_n$, respectively, with $Z^{m}_{\Lambda} (\mathbf{r}, E) = Z_{\Lambda} (\mathbf{r}_m, E) = Z_{\Lambda} (\mathbf{r} - \mathbf{R}_m, E)$ being a function centered at site $\mathbf{R}_m$. Adopting a fully relativistic formulation\textsuperscript{34,35} for Eq. (2) one gets in a natural way access to all spin-orbit induced properties as for example the anomalous and spin Hall conductivity\textsuperscript{29,32,36} or Gilbert damping parameter.\textsuperscript{18} In this case, the functions $Z^{m}_{\Lambda} (\mathbf{r}, E)$ and $J^{mn}_{\Lambda} (\mathbf{r}', E)$ stand for the regular and irregular, respectively, solutions to the single-site Dirac equation for site $n$ with the associated single-site scattering matrix $\tau^{mn}_{\Lambda\Lambda'} (E)$. The corresponding scattering path operator $\tau^{mn}_{\Lambda\Lambda'} (E)$ accounts for all scattering events connecting the sites $n$ and $n'$. Using a suitable spinor representation for the basis functions the combined quantum number $\Lambda = (\kappa, \mu)$ stands for the relativistic spin-orbit and magnetic quantum numbers $\kappa$ and $\mu$, respectively.\textsuperscript{34,35,37}

As was demonstrated by various authors\textsuperscript{27,28,38} representing the electronic structure in terms of the Green function $G^+(\mathbf{r}, \mathbf{r}', E)$ allows to account for chemical disorder in a random alloy by making use of a suitable alloy theory. In this case $\langle \ldots \rangle_c$ stands for the configurational average for a substitutional alloy concerning the site occupation. Corresponding expressions for the conductivity tensor have been worked out by Velicky\textsuperscript{27} and Butler\textsuperscript{28} using the single-site Coherent Potential Approximation (CPA) that include in particular the so-called vertex corrections.

The CPA can be used to deal with chemical but also with any other type of disorder. In fact, making use of the different time scales connected with the electronic propagation and spin fluctuations the alloy analogy is exploited when dealing with finite temperature magnetism on the basis of the disordered local moment (DLM) model.\textsuperscript{26,39} Obviously, the same approach can be used when dealing with response tensors at finite temperatures. In connection with the conductivity this is often called adiabatic approximation.\textsuperscript{40} Following this philosophy, the CPA has been used recently also when calculating response tensors using Eq. (1) with disorder in the system caused by thermal lattice vibrations\textsuperscript{15,31} as well as spin fluctuations.\textsuperscript{20,41}

B. Treatment of thermal lattice displacement

A way to account for the impact of the thermal displacement of atoms from their equilibrium positions, i.e. for thermal lattice vibrations, on the electronic structure is to set up a representative displacement configuration for the atoms within an enlarged unit cell (super-cell technique). In this case one has to use either a very large super-cell or to take the average over a set of super-cells. Alternatively, one may make use of the alloy analogy for the averaging problem. This allows in particular to restrict to the standard unit cell. Neglecting the correlation between the thermal displacements of neighboring atoms from their equilibrium positions the properties of the thermal averaged system can be deduced by making use of the single-site CPA. This basic idea is illustrated by Fig. 1. To make use of this scheme a discrete set of $N_v$ displacement vectors $\Delta \mathbf{R}_v^q (T)$ with probability $x^q_v$ ($v = 1, \ldots, N_v$) is constructed for each basis atom $q$ within
the standard unit cell that is conform with the local symmetry and the temperature dependent root mean square displacement \((\langle u^2 \rangle_T)^{1/2}\) according to:

\[
\frac{1}{N_v} \sum_{i=1}^{N_v} |\Delta R_v^i(T)|^2 = \langle u^2 \rangle_T .
\] (3)

In the general case, the mean square displacement along the direction \(\mu (\mu = x, y, z)\) of the atom \(i\) can be either taken from experimental data or represented by the expression based on the phonon calculations.\(^{42}\)

\[
\langle u^2_{i,\mu} \rangle_T = \frac{3h}{2M_1} \int_0^\infty d\omega g_{i,\mu}(\omega) \frac{1}{\omega} \coth \frac{\hbar \omega}{2k_B T} ,
\] (4)

where \(h = 2\pi \hbar\) the Planck constant, \(k_B\) the Boltzmann constant, \(g_{i,\mu}(\omega)\) is a partial phonon density of states.\(^{42}\)

On the other hand, a rather good estimate for the root mean square displacement can be obtained using Debye’s theory. In this case, for systems with one atom per unit cell, Eq. (4) can be reduced to the expression:

\[
\langle u^2 \rangle_T = \frac{1}{4} \frac{3h^2}{\pi^2} M_1 k_B \Theta_D \left[ \frac{\Phi(\Theta_D/T)}{\Theta_D/T} + \frac{1}{4} \right]
\] (5)

with \(\Phi(\Theta_D/T)\) the Debye function and \(\Theta_D\) the Debye temperature.\(^{43}\) Ignoring the zero temperature term \(1/4\) and assuming a frozen potential for the atoms, the situation can be dealt with in full analogy to the treatment of disordered alloys on the basis of the CPA. The probability \(x_v\) for a specific displacement \(v\) may normally be chosen as \(1/N_v\). The Debye temperature \(\Theta_D\) used in Eq. (5) can be either taken from experimental data or calculated representing it in terms of the elastic constants.\(^{44}\) In general the latter approach should give more reliable results in the case of multicomponent systems.

To simplify notation we restrict in the following to systems with one atom per unit cell. The index \(q\) numbering sites in the unit cell can therefore be dropped, while the index \(n\) numbers the lattice sites.

Assuming a rigid displacement of the atomic potential in the spirit of the rigid muffin-tin approximation\(^{45,46}\) the corresponding single-site t-matrix \(\mathbf{t}^\text{loc}\) with respect to the local frame of reference connected with the displaced atomic position is unchanged. With respect to the global frame of reference connected with the equilibrium atomic positions \(\mathbf{R}_n\), however, the corresponding t-matrix \(\mathbf{t}\) is given by the transformation:

\[
\mathbf{t} = \mathbf{U}(\Delta \mathbf{R}) \mathbf{t}^\text{loc} \mathbf{U}(\Delta \mathbf{R})^{-1} .
\] (6)

The so-called U-transformation matrix \(\mathbf{U}(s)\) is given in its non-relativistic form by:\(^{45,46}\)

\[
\mathbf{U}_{LL'}(s) = 4\pi \sum_{L''} \psi_{l+1}^{*\prime} Y_{l'}(\hat{s}) Y_{l''}(\hat{s}) .
\] (7)

Here \(L = (l, m)\) represents the non-relativistic angular momentum quantum numbers, \(j_l(x)\) is a spherical Bessel function, \(Y_{l'}(\hat{s})\) a real spherical harmonics, \(C_{ll'l''}\) a corresponding Gaunt number and \(k = \sqrt{\mathbf{E}}\) is the electronic wave vector. The relativistic version of the U-matrix is obtained by a standard Clebsch-Gordan transformation.\(^{37}\)

The various displacement vectors \(\Delta \mathbf{R}_v(T)\) can be used to determine the properties of a pseudo-component of a pseudo alloy. Each of the \(N_v\) pseudo-components with \(|\Delta \mathbf{R}_v(T)| = (\langle u^2 \rangle_T)^{1/2}\) is characterized by a corresponding U-matrix \(\mathbf{U}\) and t-matrix \(\mathbf{t}\). As for a substitutional alloy the configurational average can be determined by solving the multi-component CPA equations within the global frame of reference:

\[
\zeta_{CPA}^{nn} = \sum_{v=1}^{N_v} x_v \zeta_{v}^{nn}
\] (8)

\[
\zeta_{v}^{nn} = \left[ (\zeta_{v})^{-1} - (\zeta_{CPA})^{-1} + (\zeta_{CPA}^{nn})^{-1} \right]^{-1}
\] (9)

\[
\zeta_{CPA}^{nn} = \frac{1}{N_{BZ}} \int_{\Omega_{BZ}} d^3 k \left[ (\zeta_{CPA})^{-1} - \zeta_{CPA}(k, E) \right]^{-1}
\] (10)

where the underline indicates matrices with respect to the combined index \(\Lambda\). As it was pointed out in the previous work\(^{41}\), the cutoff for the angular momentum expansion in these calculations should be taken \(l \leq l_{max} + 1\) with the \(l_{max}\) value used in the calculations for the non-distorted lattice.

The first of these CPA equations represents the requirement for the mean-field CPA medium that embedding of a component \(v\) should lead in the average to no additional scattering. Eq. (9) gives the scattering path operator for the embedding of the component \(v\) into the CPA medium while Eq. (10) gives the CPA scattering path operator in terms of a Brillouin zone integral with \(\zeta_{CPA}(k, E)\) the so-called KKR structure constants.

Having solved the CPA equations the linear response quantity of interest may be calculated using Eq. (1) as for an ordinary substitutional alloy.\(^{27,28}\) This implies that one also have to deal with the so-called vertex corrections\(^{27,28}\) that take into account that one has to deal with a configuration average of the type \(\langle \mathbf{A}_\mu \mathbf{G}^+ \mathbf{A}_\nu \mathbf{G}^+ \rangle_c\) that in general will differ from the simpler product \(\langle \mathbf{A}_\mu \mathbf{G}^+ \rangle_c \langle \mathbf{A}_\nu \mathbf{G}^+ \rangle_c\).
C. Treatment of thermal spin fluctuations

As for the disorder connected with thermal displacements the impact of disorder due to thermal spin fluctuations may be accounted for by use of the super-cell technique. Alternatively one may again use the alloy analogy and determine the necessary configurational average by means of the CPA as indicated in Fig. 2. As

\[
P(\hat{c}_f) \Rightarrow \left\langle \hat{c}_f \right\rangle \Rightarrow T_{\text{loc}} \psi \sigma \left( \frac{\hat{R}(\hat{c})}{\left\langle \hat{c}_f \right\rangle} T_{\text{loc}} \right) \left( \frac{\hat{R}(\hat{c})}{\left\langle \hat{c}_f \right\rangle} T_{\text{loc}} \right)^{-1}.
\]

Figure 2. Configurational averaging for thermal spin fluctuations: the continuous distribution \( P(\hat{c}_f) \) for the orientation of the magnetic moments is replaced by a discrete set of orientation vectors \( \hat{c}_f \) occurring with a probability \( x_f \). The configurational average for this discrete set of orientations is made using the CPA leading to a periodic effective medium.

for the thermal displacements in a first step a set of representative orientation vectors \( \hat{c}_f \) (with \( f = 1, ..., N_f \)) for the local magnetic moment is introduced (see below). Using the rigid spin approximation the spin-dependent part \( B_{\text{loc}} \) of the exchange-correlation potential does not change for the local frame of reference fixed to the magnetic moment when the moment is oriented along an orientation vector \( \hat{c}_f \). This implies that the single-site t-matrix \( t_{\text{loc}} \) in the local frame is the same for all orientation vectors. With respect to the common global frame that is used to deal with the multiple scattering (see Eq. (10)) the t-matrix for a given orientation vector is determined by:

\[
t = \frac{\hat{R}(\hat{c})}{\left\langle \hat{c}_f \right\rangle} T_{\text{loc}} \frac{\hat{R}(\hat{c})}{\left\langle \hat{c}_f \right\rangle} T_{\text{loc}}^{-1}.
\]

Here the transformation from the local to the global frame of reference is expressed by the rotation matrices \( \hat{R}(\hat{c}) \) that are determined by the vectors \( \hat{c} \) or corresponding Euler angles.\(^{37}\)

Again the configurational average for the pseudo-alloy can be obtained by setting up and solving CPA equations in analogy to Eqs. (8) to (10).

D. Models of spin disorder

The central problem with the scheme described above is obviously to construct a realistic and representative set of orientation vectors \( \hat{c}_f \) and probabilities \( x_f \) for each temperature \( T \). A rather appealing approach is to calculate the exchange-coupling parameters \( J_{ij} \) of a system in an ab-initio way\(^ {25,47,48}\) and to use them in subsequent Monte Carlo simulations. Fig. 3 (top) shows results for the temperature dependent average reduced magnetic moment of corresponding simulations for bcc-Fe obtained for a periodic cell with 4096 atom sites. The full line gives the value for the reduced magnetic moment \( M_{\text{MC}}(T) = \langle m_z \rangle_T / \langle m \rangle_{T=0} \) projected on the z-axis for the last Monte Carlo step (\( \hat{z} \) is the orientation of the total moment, i.e. \( \langle \hat{m} \rangle_T \parallel \hat{z} \); the saturated magnetic moment at \( T = 0 \) K is \( m_0 = \langle \hat{m} \rangle_{T=0} \)). This scheme is called MC\(^*\) in the following. In spite of the rather large number of sites (4096) the curve is rather noisy in particular when approaching the Curie temperature. Nevertheless, the
spin configuration of the last MC step was used as an input for subsequent SPR-KKR-CPA calculations using the orientation vectors \( \hat{e}_f \) with the probability \( x_f = 1/N_f \) with \( N_f = 4096 \). As Fig. 3 (top) shows, the temperature dependent reduced magnetic moment \( M_{KKR(MC^*)}(T) \) deduced from the electronic structure calculations follows one-to-one the Monte Carlo data \( M_{MC^*}(T) \). This is a very encouraging result for further applications (see below) as it demonstrates that the CPA although being a mean-field method and used here in its single-site formulation is nevertheless capable to reproduce results of MC simulations that go well beyond the mean-field level.

However, using the set of vectors \( \hat{e}_f \) of scheme MC* also for calculations of the Gilbert damping parameters \( \alpha \) as a function of temperature led to extremely noisy and unreliable curves for \( \alpha(T) \). For that reason an average has been taken over many MC steps (scheme MC) leading to a much smoother curve for \( M_{MC^*}(T) \) as can be seen from Fig. 3 (middle) with a Curie temperature \( T_{MC}^C = 1082 \) K. As this enlarged set of vectors \( \hat{e}_f \) got too large to be used directly in subsequent SPR-KKR-CPA calculations, a scheme was worked out to get a set of vectors \( \hat{e}_f \) and probabilities \( x_f \) that is not too large but nevertheless leads to smooth curves for \( M(T) \).

The first attempt was to use the Curie temperature \( T^C_{MC} \) to deduce a corresponding temperature independent Weiss-field \( w(T_C) \) on the basis of the standard mean-field relation:

\[
w(T_C) = \frac{3k_BT_C}{m_0}.
\]

This leads to a reduced magnetic moment curve \( M_{MF}(T) \) that shows by construction the same Curie temperature as the MC simulations. For temperatures between \( T = 0 \) K and \( T_C \), however, the mean-field reduced magnetic moment \( M_{MF}(T) \) is well below the MC curve (see Fig. 3 (middle)).

As an alternative to this simple approach we introduced a temperature dependent Weiss field \( w(T) \). This allows to describe the temperature dependent magnetic properties using the results obtained beyond the mean-field approximation. At the same time the calculation of the statistical average can be performed treating the model Hamiltonian in terms of the mean-field theory. For this reason the reduced magnetic moment \( M(T) \), being a solution of equation (see e.g. 49)

\[
M(T) = L\left(\frac{w m_0^2 M(T)}{k_BT}\right),
\]

was fitted to that obtained from MC simulations \( M_{MC}(T) \) with the Weiss field \( w(T) \) as a fitting parameter, such that

\[
\lim_{w \rightarrow w(T)} M(T) = M_{MC}(T),
\]

with \( L(x) \) the Langevin function.

The corresponding temperature dependent probability \( x(\hat{e}) \) for an atomic magnetic moment to be oriented along \( \hat{e} \) is proportional to \( \exp(-w(T) \hat{e} \cdot \hat{e}/k_BT) \) (see, e.g. 49). To calculate this value we used \( N_\theta \) and \( N_\phi \) points for a regular grid for the spherical angles \( \theta \) and \( \phi \) corresponding to the vector \( \hat{e}_f \):

\[
x_f = \frac{\exp(-w(T) \hat{e}_f \cdot \hat{e}_f /k_BT)}{\sum_{f'} \exp(-w(T) \hat{e}_f \cdot \hat{e}_{f'}/k_BT)}.
\]

Fig. 4 shows for three different temperatures the \( \theta \)-dependent behavior of \( x(\hat{e}) \). As one notes, the MF-fit to the MC-results perfectly reproduces these data for all temperatures. This applies of course not only for the angular resolved distribution of the magnetic moments shown in Fig. 4 but also for the average reduced magnetic moment recalculated using Eq. (13), shown in Fig. 3. Obviously, the MF-curve \( M_{MF(MC)}(T) \) obtained using the temperature dependent Weiss field parameter \( w(T) \) perfectly reproduces the original \( M_{MC}(T) \) curve. The great advantage of this fitting procedure is that it allows to replace the MC data set with a large number...
temperature reduced magnetic moment $M(T)$ as input it can be applied not only to MC data but also to experimental data. Fig. 3 shows that the mean field fit $M_{\text{MF(exp)}}(T)$ again perfectly fits the experimental reduced magnetic moment curve $M_{\text{exp}}(T)$. Based on this good agreement this corresponding data set $\{\hat{e}_f, x_f\}$ has also been used for the calculation of response tensors (see below).

An additional much simpler scheme to simulate the experimental $M_{\text{exp}}(T)$ curve is to assume the individual atomic moments to be distributed on a cone, i.e. with $N_\theta = 1$ and $N_\phi >> 1$. \cite{23} In this case the opening angle $\theta(T)$ of the cone is chosen such to reproduce $M(T)$. In contrast to the standard DLM picture, this simple scheme allows already to account for transversal components of the magnetization. Corresponding results for response tensor calculations will be shown below.

Finally, it should be stressed here that the various spin configuration models discussed above assume a rigid spin moment, i.e. its magnitude does not change with temperature nor with orientation. In contrast to this Ruban et al. \cite{54} use a longitudinal spin fluctuation Hamiltonian with the corresponding parameters derived from ab-initio calculations. As a consequence, subsequent Monte Carlo simulations based on this Hamiltonian account in particular for longitudinal fluctuations of the spin moments. A similar approach has been used by Drehal et al. \cite{55,56} leading to good agreement with the results of Ruban et al. However, the scheme used in these calculations does not supply in a straightforward manner the necessary input for temperature dependent transport calculations. This is different from the work of Staunton et al. \cite{57} who performed self-consistent relativistic DLM calculations without the restriction to a collinear spin configuration. This approach in particular accounts in a self-consistent way for longitudinal spin fluctuations.

E. Combined chemical and thermally induced disorder

The various types of disorder discussed above may be combined with each other as well as with chemical i.e. substitution disorder. In the most general case a pseudo-component $(vft)$ is characterized by its chemical atomic type $t$, the spin fluctuation $f$ and lattice displacement $v$. Using the rigid muffin-tin and rigid spin approximations, the single-site t-matrix $t^{vft}$ combines the concentration $x_{vft}$ and lattice displacement $\Delta R_v$, and coincides with $\mathbf{L}$ for the atomic type $t$. With respect to the common global frame one has accordingly the t-matrix:

$$\mathbf{L}_{vft} = \mathbf{U}(\Delta R_v) \mathbf{R}(\hat{e}_f) \mathbf{L} \mathbf{R}(\hat{e}_f)^{-1} \mathbf{U}(\Delta R_v)^{-1}.$$  \hspace{1cm} (17)

With this the corresponding CPA equations are identical to Eqs. (8) to (10) with the index $v$ replaced by the combined index $(vft)$. The corresponding pseudo-concentration $x_{vft}$ combines the concentration $x_t$ of the
atomic type \( t \) with the probability for the orientation vector \( \hat{e}_f \) and displacement vector \( \Delta R_{vec} \).

III. COMPUTATIONAL DETAILS

The electronic structure of the investigated ferromagnets bcc-Fe and fcc-Ni, has been calculated self-consistently using the spin-polarized relativistic KKR (SPR-KKR) band structure method.\(^{58,59}\) For the exchange correlation potential the parametrization as given by Vosko et al.\(^{60}\) has been used. The angular-momentum projection cutoff of \( l_{\text{max}} = 3 \) was used in the KKR multiple scattering expansion. The lattice parameters have been set to the experimental values.

In a second step the exchange-coupling parameters \( J_{ij} \) have been calculated using the so-called Lichtenstein formula.\(^{25}\) Although the SCF-calculations have been done on a fully-relativistic level the anisotropy of the exchange coupling due to the spin-orbit coupling has been neglected here. Also, the small influence of the magneto-crystalline anisotropy for the subsequent Monte Carlo (MC) simulations has been ignored, i.e. these have been based on a classical Heisenberg Hamiltonian. The MC simulations were done in a standard way using the Metropolis algorithm and periodic boundary conditions. The theoretical Curie temperature \( T_C^{MC} \) has been deduced from the maximum of the magnetic susceptibility.

The temperature dependent spin configuration obtained during a MC simulation has been used to construct a set of orientations \( \hat{e}_f \) and probabilities \( x_f \) according to the schemes MC* and MC described in section IID to be used within subsequent SPR-KKR-CPA calculations (see above). For the corresponding calculation of the reduced magnetic moment the potential obtained from the SCF-calculation for the perfect ferromagnetic state \(( T = 0 \text{K}) \) has been used. The calculation for the electrical conductivity as well as the Gilbert damping parameter has been performed as described elsewhere.\(^{41,61}\)

IV. RESULTS AND DISCUSSION

A. Temperature dependent conductivity

Eq. (1) has been used together with the various schemes described above to calculate the temperature dependent longitudinal resistivity \( \rho(T) \) of the pure ferromagnets Fe, Co and Ni. In this case obviously disorder due to thermal displacements of the atoms as well as spin fluctuations contribute to the resistivity.

To give an impression on the impact of the thermal displacements alone Fig. 5 gives the temperature dependent resistivity \( \rho(T) \) of pure Cu \(( \Theta_{\text{Debye}} = 315 \text{ K}) \) that is found in very good agreement with corresponding experimental data.\(^{62}\) This implies that the alloy analogy model that ignores any inelastic scattering events should in general lead to rather reliable results for the resistivity induced by thermal displacements. Accordingly, comparison with experiment should allow for magnetically ordered systems to find out the most appropriate model for spin fluctuations.

Fig. 6 (top) shows theoretical results for \( \rho(T) \) of bcc-Fe due to thermal displacements \( \rho_v(T) \), spin fluctuations described by the scheme MC \( \rho_{MC}(T) \) as well as the combination of the two influences \( (\rho_v,MC(T)) \). First of all one notes that \( \rho_v(T) \) is not influenced within the adopted model by the Curie temperature \( T_C \) but is determined only by the Debye temperature. \( \rho_{MC}(T) \), on the other hand, reaches saturation for \( T_C \) as the spin disorder does not increase anymore with increasing temperature in the paramagnetic regime. Fig. 6 also shows that \( \rho_v(T) \) and \( \rho_{MC}(T) \) are comparable for low temperatures but \( \rho_{MC}(T) \) exceeds \( \rho_v(T) \) more and more for higher temperatures. Most interestingly, however, the resistivity for the combined influence of thermal displacements and spin fluctuations \( \rho_{v,MC}(T) \) does not coincide with the sum of \( \rho_v(T) \) and \( \rho_{MC}(T) \) but exceeds the sum for low temperatures and lies below the sum when approaching \( T_C \).

Fig. 6 (bottom) shows the results of three different calculations including the effect of spin fluctuations as a function of the temperature. The curve \( \rho_{MC}(T) \) is identical with that given in Fig. 6 (top) based on Monte Carlo simulations. The curves \( \rho_{DLM(MC)}(T) \) and \( \rho_{cone(MC)}(T) \) are based on a DLM- and cone-like representation of the MC-results, respectively. For all three cases results are given including as well as ignoring the vertex corrections. As one notes the vertex corrections play a negligible role for all three spin disorder models. This is fully in line with the experience for the longitudinal resistivity of disordered transition metal alloys: as long as the the states at the Fermi level have dominantly d-character the vertex corrections can be neglected in general. On the other hand, if the sp-character domi-
Comparing the DLM-result $\rho_{\text{DLM}(MC)}(T)$ with $\rho_{\text{MC}}(T)$ one notes in contrast to the results for $M(T)$ shown above (see Fig. 3 (bottom)) quite an appreciable deviation. This implies that the restricted collinear representation of the spin configuration implied by the DLM-model introduces errors for the configurational average that seem in general to be unacceptable. For the Curie temperature and beyond in the paramagnetic regime $\rho_{\text{DLM}(MC)}(T)$ and $\rho_{\text{MC}}(T)$ coincide, as it was shown formally before.\textsuperscript{20}

Comparing finally $\rho_{\text{cone}(MC)}(T)$ based on the conical representation of the MC spin configuration with $\rho_{\text{MC}}(T)$ one notes that also this simplification leads to quite strong deviations from the more reliable result. Nevertheless, one notes that $\rho_{\text{DLM}(MC)}(T)$ agrees with $\rho_{\text{MC}}(T)$ for the Curie temperature and also accounts to some extent for the impact of the transversal components of the magnetization.

The theoretical results for bcc-Fe ($\Theta_\text{Debye} = 420$ K) based on the combined inclusion of the effects of thermal displacements and spin fluctuations using the MC scheme ($\rho_{\text{MC}}(T)$) are compared in Fig. 7 (top) with experimental data ($\rho_{\text{exp}}(T)$). For the Curie temperature ob-
\( \rho_{\text{exp}}(T) \) can be attributed to the longitudinal spin fluctuations leading to a temperature dependent distribution of local magnetic moments on Fe atoms.\(^{54}\) However, this contribution was not taken into account because of restriction in present calculations using fixed value for the local reduced magnetic moments.

Fig. 7 (bottom) shows corresponding results for the temperature dependent resistivity of fcc-Ni (\( \Theta_{\text{Debye}} = 375 \) K). For the ferromagnetic (FM) regime that the theoretical results are comparable in magnitude when only thermal displacements (\( \rho_{\alpha}(T) \)) or spin fluctuations (\( \rho_{\text{MF}}(T) \)) are accounted for. In the later case the mean field \( w(T) \) has been fitted to the experimental \( M(T) \)-curve. Taking both into account leads to a resistivity \( \rho_{\alpha,\text{MF}}(T) \) that are well above the sum of the individual terms \( \rho_{\alpha}(T) \) and \( \rho_{\text{MF}}(T) \). Comparing \( \rho_{\alpha,\text{MF}}(T) \) with experimental data \( \rho_{\text{exp}}(T) \) our finding shows that the theoretical results overshoots the experimental one the closer one comes to the critical temperature. This is a clear indication that the assumption of a rigid spin moment is quite questionable as the resulting contribution to the resistivity due to spin fluctuations as much too small. In fact the simulations of Ruban et al.\(^{54}\) on the basis of a longitudinal spin fluctuation Hamiltonian led on the case of fcc-Ni to a strong diminishing of the average local magnetic moment when the critical temperature is approached from below (about 20 \% compared to \( T = 0 \) K).

For bcc-Fe, the change is much smaller (about 3 \%) justifying on the case the assumption of a rigid spin moment. Taking the extreme point of view that the spin moment vanishes completely above the critical temperature or the paramagnetic (PM) regime only thermal displacements have to be considered as a source for a finite resistivity. Corresponding results are shown in Fig. 7 (bottom) together with corresponding experimental data. The very good agreement between both obviously suggests that remaining spin fluctuations above the critical temperature are of minor importance for the resistivity of fcc-Ni.

### B. Temperature dependent Gilbert damping parameter

Fig. 8 shows results for Gilbert damping parameter \( \alpha \) of bcc-Fe obtained using different models for the spin fluctuations. All curves show the typical conductivity-like behavior for low temperatures and the resistivity-like behavior at high temperatures reflecting the change from dominating intra- to inter-band transitions.\(^{66}\) The curve denoted expt is based on a spin configuration toted to the experimental \( M_{\text{exp}}(T) \) data. Using the conical model to fit \( M_{\text{exp}}(T) \) as basis for the calculation of \( \alpha(T) \) leads obviously to a rather good agreement with \( \alpha_{M_{\text{exp}}}^{(T)} \). Having instead a DLM-like representation of \( M_{\text{exp}}(T) \), on the other hand, transverse spin components are suppressed and noteworthy deviations from \( \alpha_{M_{\text{exp}}}^{(T)} \) are found for the low temperature regime. Nevertheless, the deviations are less pronounced than in the case of the longitudinal resistivity (see Fig. 6 (bottom)), where corresponding results are shown based on \( M_{\text{MC}}(T) \) as a reference. Obviously, the damping parameter \( \alpha \) seems to be less sensitive to the specific spin fluctuation model used than the resistivity. Finally, using the spin configuration deduced from Monte Carlo simulations, i.e. based on \( M_{\text{MC}}(T) \) quite strong deviations for the resulting \( \alpha_{M_{\text{MC}}}^{(T)} \) from \( \alpha_{M_{\text{exp}}}^{(T)} \) are found. As for the resistivity (see Fig. 6 (bottom)) this seems to reflect the too fast drop of the reduced magnetic moment \( M_{\text{MC}}(T) \) with temperature in the low temperature regime compared with temperature (see Fig. 3). As found before\(^{18}\) accounting only for thermal vibrations \( \alpha(T) \) (Fig. 6 (bottom)) is found comparable to the case when only thermal spin fluctuations are allowed. Combing both thermal effects does not lead to a curve that is just the sum of the two \( \alpha(T) \) curves. As found for the conductivity (Fig. 6 (top)) obviously the two thermal effects are not simply additive. As Fig. 9 (top) shows, the resulting damping parameter \( \alpha(T) \) for bcc-Fe that accounts for thermal vibrations as well as spin fluctuations is found in reasonable good agreement with experimental data.\(^{18}\)

Fig. 9 shows also corresponding results for the Gilbert damping of fcc-Ni as a function of temperature. Accounting only for thermal spin fluctuations on the basis of the experimental \( M(T) \)-curve leads in this case to completely unrealistic results while accounting only for thermal displacements leads to results already in rather good agreement with experiment. Taking finally both sources of disorder into account again no simple additive behavior is found but the results are nearly unchanged compared to those based on the thermal displacements alone. This implies that results for the Gilbert damping parameter of fcc-Ni hardly depend on the specific spin configuration model used but are much more governed by thermal displacements.
properties relevant in spintronics have been presented and discussed. Technical details of an implementation within the framework of the spin-polarized relativistic KKR-CPA band structure method have been outlined that allow to deal with thermal vibrations as well as spin fluctuations. Various models to represent spin fluctuations have been compared with each other concerning corresponding results for the temperature dependence of the reduced magnetic moment $M(T)$ as well as response quantities. It was found that response quantities are much more sensitive to the spin fluctuation model as the reduced magnetic moment $M(T)$. Furthermore, it was found that the influence of thermal vibrations and spin fluctuations is not additive when calculating electrical conductivity or the Gilbert damping parameter $\alpha$. Using experimental data for the reduced magnetic moment $M(T)$ to set up realistic temperature dependent spin configurations satisfying agreement for the electrical conductivity as well as the Gilbert damping parameter could be obtained for elemental ferromagnets bcc-Fe and fcc-Ni.

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**V. SUMMARY**

Various schemes based on the alloy analogy that allow to include thermal effects when calculating response
