Ultrafast dynamics in ferrimagnetic materials with a quantum Monte Carlo atomistic model

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We investigate the ultrafast dynamics of the atomic angular momentum in ferrimagnets irradiated by laser pulses. Our study is based on a quantum atomistic approach and the particle dynamics is performed using a Monte Carlo technique. We focus on microscopic mechanisms that lead to the dissipation of the total angular momentum in a rare earth–transition metal (RE-TM) alloy in which the two sublattices have opposite spin orientation. We describe the coherent transfer of atomic angular momentum between the spin and the orbital momentum. The orbital momentum quenching induced by the lattice field and the Elliott-Yafet collision mechanism are also included. The simulations show that the observed ultrafast magnetization quenching may be explained at a microscopic level by the combined effects of the coherent spin transfer between the RE and the TM sublattices along with the quenching of the localized orbital angular momentum induced by the lattice field.

DOI: 10.1103/PhysRevB.96.024441

I. INTRODUCTION

The study of ultrafast magnetization dynamics of nanostructures has emerged as being a rich and active multidisciplinary discipline of theoretical and experimental physics. Since the discovery by Beaurepaire et al. [1] in 1996 of the femtosecond ultrafast demagnetization in magnetic metals induced by laser, the study of time-dependent magneto-optical effects related to spin and charge excitations along with their various relaxation processes has stimulated recently an intense research activity.

The first phenomenological model that has been suggested to quantify the exchange energy processes in a magneto-optical experiment is the so-called three temperature model (TTM) [1]. According to this model, the atomic spin, the energy bands of the electrons, and the phonon bath are considered as three macroscopic reservoirs that exchange energy and angular momentum. The infrared femtosecond laser pulse injects energy in the magnetic material by perturbing the electron distribution in the vicinity of the Fermi level [2,3]. In a time scale of few hundred femtoseconds, the energy is transferred to the lattice and to the spins by electron-phonon collisions and by spin-spin interactions. The increase of the spin temperature is confirmed by the observation of the ultrafast magnetization quenching of the sample. The three-temperature model does not address the specific question of angular momentum conservation at the femtosecond time scale. In spite of intensive investigations, the microscopic origin of the ultrafast demagnetization remains controversial [4].

Several microscopic mechanisms have been proposed to characterize the spin-flip channel which is responsible for the dissipation of the spin angular momentum on a time scale of few hundred femtoseconds. The phenomena that have received particular attention are the direct coupling between the electron spins and the laser electrical field [5,6], the electron-magnon scattering process [7], the defect- and phonon-induced Elliott-Yafet spin flips [8,9], the ultrafast quenching of the magnetocrystalline anisotropy [10], and finally, the superdiffusive spin transport [11,12]. Even if all those mechanisms were sustained by experimental evidences, interrogations still remain concerning their actual efficiency [13,14].

Ab initio calculations based on many-body theories [15,16], and on-time-dependent Kohn-Sham density functional theory (TDDFT) [17] indicate that the spin-orbit interaction plays a central role in the description of the demagnetization process of few transition metals. However, due to the high computational cost, direct TDDFT calculations suffer from serious limitations. Indeed, they are restricted to simple structures and the incorporation of phonon processes goes beyond today’s computational capabilities.

Ferrimagnetic alloys are ideal systems where the transfer of spin and angular momentum between valence and conduction electrons can be investigated. The most common ferrimagnetic alloys are formed by a sublattice of transition-metal (TM) atoms coupled with a sublattice of rare-earth (RE) atoms oriented with opposite spin direction. Typical elements are Fe [18,19], Co [20], and Pd [21] for the transition metals, and Gd [18,19,22] and Tb [23] for the rare-earth elements.

The magnetization quenching time scale in monoatomic films excited by short laser pulses is different for TM [1,24] and RE [25,26] atoms. This difference has been attributed to the nature of the orbitals that carry the magnetic moment. In the case of TM films, the magnetism is due to $3\text{d}$ itinerant electrons that are directly excited by the laser pulse. In the case of RE, the magnetism is due to $4\text{f}$ localized electrons whose excitation is mediated through the $5\text{d}$-$4\text{f}$ exchange coupling [27].

The investigation of ultrafast magnetization dynamics in TM-RE alloys would provide useful information about the transfer of angular momentum in coupled systems. The ultrafast magnetization dynamics in RE-TM has been reproduced by atomistic models [14,18,19,28]. However, the numerical results are very sensitive to the values of the exchange constants that are usually free parameters of the model. Moreover, the itinerant character of the $3\text{d}$-band electrons cannot be reproduced by the standard atomistic methods. The latter are based on the phenomenological Landau-Lifshitz-Gilbert (LLG) equation in which the atomic angular momentum is modeled by a classical vector. Since quantum properties of
the electron spin are neglected, the validity of the atomistic models based on the classical LLG equation which is used for studying the magnetic properties of nanometric systems is questionable.

In this contribution, we propose a quantum atomistic approach for the spin dynamics of a system of interacting atoms. Our model describes the coherent exchange of spin and orbital angular momentum among the atoms and includes the major sources of dissipation of the angular momentum, such as the interaction of the atoms with the phonon bath and the quenching of the orbital angular momentum. We have checked the ability of our model to reproduce the correct spin dynamics in a nanomaterial by simulating the ultrafast evolution of the magnetization observed recently in ferrimagnetic CoTb films [23].

II. MODEL

The magnetic configuration of complex materials such as RE-TM alloys can be understood by analyzing the local-local (on-site) interactions and the interactions between localized and itinerant electrons. The magnetism of RE elements is due, to a greater extent, to the localized \( f \) orbitals, while in TM elements the dominant contribution to the magnetism comes from the \( d \) orbitals which have a mixed localized-itinerant character.

Our model describes localized orbitals as well as itinerant electrons. In order to illustrate our method, we consider a prototype of a RE-TM material which is composed by only two types of orbitals, the localized (\( f \)-type) and the itinerant (\( d \)-type). Such a classification in strictly localized or delocalized electrons is a simple idealization. In reality, localized and delocalized orbitals mix to some extent. For this reason, in our simulations we have considered a more realistic model where \( d \) orbitals in cobalt have a mixed localized-itinerant character.

Localized electrons describe inner orbitals that do not participate in electron transport. The electrons around one atomic site are considered as a single quantum object with total spin \( S \). Delocalized electrons are characterized by a spin \( 1/2 \), a momentum \( k \), and are described by a continuous distribution function. More precisely, local electrons depict the projection of the many-electron wave function in a small domain close to the atomic positions.

It is convenient to distinguish between interatomic and local processes. We denote by interatomic processes the phenomena in which localized and delocalized electrons exchange spin and energy with the surrounding atoms and with the phonon bath. The remaining (local) processes concern the local exchange of spin and angular momentum. We also include spin-orbit interaction and the orbital quenching induced by the lattice field.

Experiments as well as theoretical models indicate that the spin-orbit interaction may play a central role on the evolution of the atomic spin in solids [13,17,29,30]. Indeed, spin-orbit interaction is relevant to understanding the most famous mechanisms of dissipation of the total angular momentum of the electrons such as the Elliott-Yafet, Dyakonov-Perel, the Rashba, and the Gilbert damping effect. In particular, we focus on the transfer of momentum between spin and orbital degrees of freedom in a strongly out-of-equilibrium regime. This issue is rather unexplored.

First, we treat the local processes. The local Hamiltonian takes the form

\[
\mathcal{H}(\mathbf{R}_i) = \lambda_{SO} \mathbf{L}_i \cdot \mathbf{S}_i + \sum_{j \in NA_i} \gamma_{ij} \mathbf{S}_j + V,
\]

where \( \mathcal{H}(\mathbf{R}_i) \) is the atom Hamiltonian at position \( \mathbf{R}_i \). The first term of the equation is the spin-orbit interaction. It is responsible for mixing the spin and the orbital momentum. The coefficient \( \lambda_{SO} \) is the spin-orbit strength and \( \mathbf{S}_i, \mathbf{L}_i \) are, respectively, the local spin and orbital momentum operators. The second term of Eq. (1) accounts for the spin exchange interaction. This term indicates that the atom at the position \( \mathbf{R}_i \) feels an effective magnetic field proportional to the value of the spin of the atom at \( \mathbf{R}_j \), weighted by the exchange interaction coefficient \( \gamma_{ij} \). The sum runs over the neighbors of the \( i \)th atom (\( NA_i \)).

The last term of Eq. (1) describes the electrostatic crystal field. It is at the origin of the quenching of the atomic orbital angular momentum. The spin-orbit interaction tends to align the spin with the orbital motion of the electrons. This mechanism competes with the orbital quenching induced by the crystal field. The lattice field interaction of various 3d TM crystals is much stronger than the spin-orbit interaction. As a result, the orbital momentum is quenched (\( L_z = 0 \)). However, in heavier TM compounds (the 4d and 5d series) the effect of the crystal field is of the same order of magnitude as the spin-orbit interaction and the orbital momentum may not be completely quenched. We model the crystal lattice potential by a cubic lattice. In this case the first correction to the spherical potential is given by the potential \( V = \lambda_1 (x^4 + y^4 + z^4) \). The strength of such a molecular field is quantified by the parameter \( \lambda_1 \). A nonspherical crystal potential induces the quenching of the orbital motion of the electrons and plays an important role in the demagnetization processes. This can be understood by the following arguments. Without \( V \), the Hamiltonian of Eq. (1) does not depend on the real-space coordinates and preserves the spherical atomic symmetry. In this case, the angular dependence of the eigenvector of \( \mathcal{H}(\mathbf{R}_i) \) is given by the spherical harmonics \( Y^m_l(\mathbf{r} - \mathbf{R}_i) \), where \( l \) is the orbital angular momentum and \( m \) the magnetic quantum number. The presence of the term \( V \) mixes the \( m \) components of the atomic wave function (as an example, \( \langle Y^2_2(\mathbf{R}_i) | V | Y^{-2}_2(\mathbf{R}_i) \rangle \approx 0.095 \lambda_1 \)). In this case, the angular momentum is no longer a good quantum number and the atomic eigenfunctions are a mixture of spherical harmonics with opposite magnetic quantum number. When the term \( V \) becomes dominant, the expectation value of the angular moment operator \( \mathbf{L} \) goes to zero (quenching of the orbital momentum).

We note that according to our classification of local and interatomic processes, in Eq. (1), the only interaction of the \( i \)th atom with the surrounding atoms comes from the molecular exchange field \( \sum_j \gamma_{ij} \mathbf{S}_j \). In order to reproduce the full many-body dynamics, we complete the description of the system by including the interaction of the localized electrons with the itinerant electrons and with the phonons (interatomic processes).

We represent the atom wave function in the product space of the spin and the orbital momentum degree of freedom (we assume a fixed quantization axis). We denote by \( \rho_{nm} \) the density matrix of the electrons in the localized orbital at the
position \( \mathbf{R}_i \), where \( m, m' (l, l') \) is the spin (orbital momentum) projection. The relevant equation for \( \rho \) is

\[
\frac{\partial \rho_{m,l,m',l'}(\mathbf{R}_i,t)}{\partial t} = -i\hbar [\mathcal{H}(\mathbf{R}_i), \rho] + \frac{\partial \rho}{\partial t}_{\text{col}}. \tag{2}
\]

The interatomic interactions are described by the last term of the von Neumann equation (2). We model the interatomic processes by means of instantaneous collisions (Markov processes). They are described by two additional Boltzmann master equations for the itinerant and localized electron densities:

\[
\frac{\partial \rho_{m,l}(\mathbf{R}_i,t)}{\partial t} = \Gamma_{\text{loc-it}}^{\sigma} - \Gamma_{\text{it-loc}}^{\sigma} \rho_{m,l} + \frac{1}{\tau_{\text{loc-it}}} \rho_{m,l}, \tag{3}
\]

\[
\frac{\partial \rho_{m,l}(\mathbf{R}_i,t)}{\partial t} = \Gamma_{\text{it-loc}}^{\sigma} + \Gamma_{\text{loc-it}}^{\sigma} \rho_{m,l} - \frac{1}{\tau_{\text{it-loc}}} \rho_{m,l}. \tag{4}
\]

We denote by \( f_{\sigma}(\mathbf{k}, \mathbf{r}) \) the density of itinerant electrons at the position \( \mathbf{r} \) with spin \( \sigma \) (\( \sigma = \uparrow, \downarrow \)) and momentum \( \mathbf{k} \), and by \( n_m(\mathbf{R}) \equiv \sum_l \rho_{m,l}(\mathbf{R}) \) the \( m \)th diagonal element of the atomic density matrix. In view of the application of the Monte Carlo (MC) solver technique, we have written the master equations in terms of loss and gain operators. The gain operators are denoted by the symbol \( \Gamma \). They describe the microscopic processes that increase the local spin density. The remaining operators, the loss terms, have the form of simple relaxation-time operators. In this way, the collision frequency \( \tau^{-1} \) associated with the interaction processes appears explicitly. As will be discussed in the following, the collision frequencies play a central role in the numerical MC scheme applied to Eqs. (3) and (4). The exchange of spin between localized and itinerant electrons is described by the operators \( \Gamma_{\text{loc-it}}^{\sigma} \) and \( \Gamma_{\text{it-loc}}^{\sigma} \) for the localized orbital and the itinerant charges, respectively.

\[
\Gamma_{\text{loc-it}}^{\sigma}(\mathbf{R}_i) = \int_{\text{FBZ}} \left( n_{m+1} w_{m+1}^{\text{m+1},m+1} + n_{m-1} w_{m}^{m-1,m} \right) \frac{d\mathbf{k}}{(2\pi)^3},
\]

\[
\Gamma_{\text{it-loc}}^{\sigma}(\mathbf{R}_i, \mathbf{k}) = \sum_m n_{m+1} w_{m+1}^{m+1,m},
\]

\[
\Gamma_{\text{loc-it}}^{\sigma}(\mathbf{R}_i, \mathbf{k}) = \sum_m n_{m-1} w_{m}^{m-1,m}.
\]

where \( w_m^{m'} = \frac{\gamma}{\pi} [S(S + 1) - m(m \pm 1)], S \) is the total spin, \( \gamma \) is the exchange interaction, FBZ indicates the first Brillouin zone, and

\[
\mathcal{T}_{\sigma,\sigma'}^{m,m'} = 2\pi \int_{\text{FBZ}} \left[ 1 - f_{\sigma}(\mathbf{k}) \right] f_{\sigma'}(\mathbf{k}') \times \delta(\varepsilon_{\sigma'} - \varepsilon_{\sigma}) \frac{d\mathbf{k}'}{(2\pi)^3}. \tag{5}
\]

Finally, we include in our model the Elliott-Yafet (EY) electron-phonon interaction with and without spin conservation [31–33]. Such collision terms are described by the scattering kernel \( \Gamma_{\text{it-ph}}^{\sigma} \) and \( \Gamma_{\text{ph-loc}}^{\sigma} \). Their expressions are given in the Appendix.

We solve the coupled von Neumann–Boltzmann (2)–(3) system by applying a MC approach. In order to illustrate our MC technique, we calculate the dynamics of the density matrix \( \rho \) by including only the collisions with the itinerant electrons. The other processes are treated in the same way.

According to the MC procedure and Eq. (3), the probability that during the time interval \( t \) the \( i \)th atom will not collide is

\[
P = e^{-\frac{t}{\tau}} \text{ where } \tau^{-1} = \sum_m 1/\tau_{\text{loc-it}}(\mathbf{R}_i) \tag{36}. \]

By sampling the distribution \( P \), we generate a set of random numbers \( r(t, \mathbf{R}_i) \). We interpret \( t^* \) as the time at which the atom at position \( \mathbf{R}_i \) collides with an itinerant electron. We solve the coherent part of the evolution equation [Eq. (2) without the last term] from the initial time \( t_0 \) to \( t^* \). The diagonal elements of the density matrix \( \rho_{m,l,m',l'}(\mathbf{R}_i,t^*) \) give the probability that at the time \( t^* \) the \( i \)th atomic spin and orbital momentum are \( m \) and \( l \), respectively. We model the collision as an instantaneous measurement of the quantum-mechanical state of the localized electrons. We select one of the possible values of the pair \((m,l)\) by generating random numbers with probability \( \rho_{m,l,m',l'}(t^*) \).

We denote by \((m^*,l^*)\) such values. After the collision, the final state will be either \((m^*+1,l^*-1)\) or \((m^*-1,l^*+1)\) with probability proportional to \(1/\tau_{\text{loc-it}}\) and to \(1/\tau_{\text{loc-it}}\), respectively. This procedure is repeated for all the atoms of the system.

### III. Results

The ultrafast dynamics of spin and orbital angular momentum in a nanostructure triggered by laser pulses is today a matter under active consideration. In the case of composite materials, such as the ferrimagnets, experiments based on the time-resolved x-ray magnetic circular dichroism are able to distinguish the evolution of the magnetization of each sublattice. This opens the possibility to investigate the exchange of spin between \( d \) and \( f \) orbitals in a TM-RE alloy and, at the same time, the transfer of angular momentum between spin and orbital angular momentum. We simulate the ultrafast evolution of spin and orbital angular momentum in a Co_{74}Tb_{26} alloy excited by a femtosecond x-ray laser pulse. We compare our results with the measurements that have been recently performed by Bergérard et al. [23]. We consider a cube of Co_{74}Tb_{26} containing around 6 \times 10^4 atoms of Co and 2 \times 10^4 atoms of Tb. The parameters required by our model may be obtained by performing static density functional theory (DFT)
FIG. 1. Ultrafast evolution of the spin (blue curve) and orbital angular momentum (red curve) after laser excitation for cobalt (left panel) and terbium (right panel). The dashed curves are obtained by imposing the conservation of total angular momentum of the system. The inset in the right panel depicts the zoom of the results for small times.

calculations [35]. The Co_{74}Tb_{26} alloy is an amorphous material and the samples are formed by disordered microcrystals. Under such conditions the DFT calculations become extremely complex and have low reliability. As mentioned in the Introduction, we attribute to the $d$ orbitals of cobalt a mixed localized-delocalized character. We assume that for each atomic Co site are present on average one localized electron and one delocalized electron. Accordingly, we model the cobalt atoms by a lattice of local electrons plus the distribution function $f_\sigma$ which describes delocalized charge. The exchange parameters used in our simulations are found by fitting the static magnetization of the alloy (Curie temperature 700 K and compensation temperature 500 K, measured in [36]). We obtain $\gamma_{Co-Tb} = -6$ meV/bound, $\gamma_{Co-Co} = 12$ meV/bound, and $\gamma_{Tb-Tb} = 1$ meV/bound. Concerning the band structure of the delocalized $d$ orbitals, we used the profile of the density of states obtained by DFT calculations for pure Co and Tb [37]. Finally, the $\lambda$ parameters that appear in Eq. (1) are obtained by reproducing the measured static mean value of the orbital angular momentum of Co and Tb. We found $\lambda_{Co} = 25$ meV for Co and for Tb $\lambda_{Tb} = 1$ meV. For the spin-orbit interaction we used $\lambda_{Co}^{SO} = 20$ meV, $\lambda_{Tb}^{SO} = 100$ meV.

In order to fix the initial magnetic configuration of the solid, we consider that for $t = 0$ the system is at equilibrium at temperature $T = 100$ K. We assume that the energy of the laser field is transferred to the solid by thermal excitation of the TM itinerant electrons. We discard the direct coupling between the charges and the photons of the laser field [6]. We assume that the laser pulse instantaneously increases the temperature of the $d$ band electrons of cobalt. We choose the initial temperature equal to 1500 K, which is far above the Curie temperature [1,19].

The evolution of the spin and orbital angular momentum of the two sublattices is depicted in Fig. 1. The full curves describe the evolution of the total spin (blue curves) and of the orbital momentum (red curves). The left (right) panel refers to the cobalt (terbium) sublattice. The evolution of the total angular momentum is depicted in Fig. 2. In the upper panel we display the angular momentum (spin plus orbital momentum) of the alloy and in the bottom panel we plot the cobalt (red curve) and terbium (blue curve) components. In agreement with the experimental results [23], our simulations show that the laser excitation induces ultrafast transfer of spin between the RE and the TM sublattices. The total magnetization of the system is quenched with a decay time of 200 fs.

The quenching of the spin polarization in ferrimagnetic alloys proceeds generally faster than in ferromagnetic systems. The spin is easily exchanged between sublattices with opposite spin polarization. In fact, in this case the spin-flip process requires only majority spins. In our case, the majority spins of the TM sublattice (down) make a spin flip with the majority spins of the RE sublattice which are directed in the opposite

FIG. 2. Upper panel: Total angular momentum of the alloy. Lower panel: Ultrafast evolution of the total angular momentum (spin plus orbital momentum) for cobalt (red curve) and terbium (blue curve). The continuous curves refer to the full solution and the dashed curves refer to the case with conservation of the total angular momentum.
direction (up). Such a spin-flip process decreases the spin polarization of both TM and RE sublattices and conserves the total spin of the system. Conservative transfer of spin is found to be faster than other spin-flip processes that demand some dissipation of the angular momentum.

In our model we include two processes that do not conserve the total angular momentum: the EY electron-phonon interaction in which the spin of the itinerant electrons is not conserved and the orbital quenching of the localized orbitals. By comparing the magnetization dynamics of Tb and Co with the time evolution of the total angular momentum of the system, Bergeard et al. suggested that the RE-TM spin exchange is not necessarily associated to the quenching of the total angular momentum. In order to investigate this statement, we have performed simulations in which we have removed the processes that do not conserve the total angular momentum. In this case the total angular momentum of the system is exactly conserved.

The results are displayed in Figs. 1 and 2 (dashed curves). Concerning the spin dynamics, our simulations show that during the first 200 fs the angular dissipation processes are not relevant. The spin dynamic in the conservative case is essentially the same as in the nonconservative one. A different conclusion is found for the dynamics of the Td orbital angular momentum. For this quantity, nonconservative effects cannot be neglected.

The results of our simulations can be interpreted as follows. The laser increases the kinetic energy of the $d$ electrons of cobalt. The hot electrons transfer energy to the RE electrons by exchanging spins. As a consequence, the spin polarization of the localized $f$ electrons of terbium decreases. The excess of energy is transferred from the spin to the orbital momentum via the SO interaction. The orbital momentum is efficiently dissipated by orbital quenching. In particular, our simulations show that in the absence of orbital quenching, initially the orbital momentum increases (see insets of Fig. 1). This is the signature of the transfer of momentum between spin and orbital angular momentum. In the conservative case, the orbital momentum behaves as a reservoir of angular momentum. The polarization is transferred back to the spin system in a longer time scale.

After the laser excitation, the ultrafast quenching is observed in both spin and orbital angular momentum [10,24]. Consequently, it is typically concluded that despite the presence of the spin-orbit coupling there is not transfer of angular momentum between spin and orbital angular momentum. Our simulations help to clarify this point. We showed that the spin-orbit coupling activates the transfer of angular momentum between the spin and orbital degree of freedom in the very early stage of the dynamics. However, due to the quenching of the orbital momentum, the increase of the orbital momentum cannot be observed within the experimental time resolution.

In conclusion, we have developed a quantum model that describes the time evolution of the spin and the orbital angular momentum of $d$ and $f$ electrons in a magnetic composite material. Our results are in good agreement with the ultrafast dynamics of the magnetization observed in ferrimagnetic alloy. Our model is able to discriminate between the spin and the orbital components of the total angular momentum. We observe that the quenching of the local orbital momentum is the main channel of dissipation of the angular momentum during the early stage of the magnetization dynamics.

ACKNOWLEDGMENTS

We thank C. Boeglin, N. Bergeard, and O. Bengone for many useful discussions. We thank the Agence Nationale de la Recherche (project Labex “Nanostructures in Interaction with their Environment”) for financial support.

APPENDIX: ELECTRON-PHONON INTERACTION

The electron-phonon collision is described by $\Gamma_{i\text{-}ph}$ and $\Gamma_{\alpha\text{-}ph}$ of Eqs. (3) and (4). We write $\Gamma_{i\text{-}ph} = \Gamma_{\alpha} + \Gamma_{\beta}$ where the abbreviations “em” and “ab” denote the phonon emission and absorption processes, respectively. We have (for a similar model see Ref. [14])

$$\Gamma_{\alpha}(k, \mathbf{r}) = 2\pi D \int_{F_{\text{BZ}}} |k - k'| \left[ 1 - f(\alpha(k)) f(\alpha(k')) \right] \times \frac{d\mathbf{k}'}{2\pi^3},$$

where $f_{\text{BE}}$ is the Bose-Einstein distribution function, $\omega$ the phonon frequency, and $D$ is the deformation potential [32]. The absorption term is obtained by making the substitution $\omega \rightarrow -\omega$, $f_{\text{BE}} + 1 \rightarrow f_{\text{BE}}$. Finally, the mean electron-phonon collision time is given by

$$\frac{1}{\tau_{\alpha}(k)} = 2\pi D \int_{F_{\text{BZ}}} |k - k'| \left[ 1 - f(\alpha(k')) \right] \times \left[ N(k - k') + 1 \right] \delta[E_{\alpha}(k) - E_{\alpha}(k') + \omega] \frac{d\mathbf{k}'}{(2\pi)^3}.$$


