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Theory of the Spin Relaxation of Conduction Electrons in Solid and Liquid Metals

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A formula for the spin-relaxation time (SRT) of conduction electrons in solid metals, obtained previously from a heuristic extension to solids of a theory proposed for liquid metals, is rigorously derived here. In this theory, which is equivalent to Yafet's within the one-phonon approximation, the SRT is expressed in terms of the dynamical-structure factor of the metal which includes the actual spectrum of lattice excitations and automatically takes into account the umklapp processes exactly. The SRT of solid sodium and potassium are calculated as a function of temperature using a simple model for the structure factor. The results are compared with available experimental data and the agreement is found to be good down to about 40 °K. Comments on the origin of the discrepancy below this temperature are made. The enhancement effect of the electron-electron interaction on the SRT is discussed.

I. INTRODUCTION

A theory of the spin-relaxation time (SRT) T_1 of conduction electrons in liquid metals proposed by Helman[1] has been used to interpret conduction-electron–spin-resonance (CESR) linewidth measurements in molten sodium by Devine and Dupree.[2] In the same paper the authors suggested a modification of the theory to be applied to solids, and with this they succeeded in explaining the temperature dependence of T_1 in solid sodium too. The formula proposed for solid metals was obtained by analogy with resistivity calculations performed by Greene and Kohn[3] (hereafter referred to as GK). In this paper we derive that result rigorously (Sec. II).[4]

Later, the theory was applied to molten potassium.[5] Its proposed extension could not be tested in solid potassium, however, owing to the lack of information about the dynamical-structure factor necessary to carry out the calculations.

Recently, the theory has been generalized to liquid-metal alloys[6] and applied to the interpretation of CESR linewidth measurements in liquid Na-K alloys in the whole concentration range.[7]

The last and most comprehensive treatise on the theory of spin-lattice relaxation of conduction electrons in solid metals is that of Yafet.[8] He derived a general expression for the spin-flip transition-matrix element and, from its dependence on the momentum transfer $\vec{q}$, he was able to show that the temperature dependence of T_1^{-1} must be analogous to that of the resistivity. However, in order to carry through a calculation of T_1, the general expression has to be simplified by approximations in the phonon spectrum and in the treatment of the umklapp processes which finally lead to the introduction of three adjustable parameters. In this form Yafet's theory has been successfully used to interpret experimental results in sodium.[8–10] Using the present approach, the difficulties leading to the introduction of adjustable parameters are overcome by expressing T_1 in terms of the dynamical-structure factor of the metal which includes the actual spectrum of lattice excitations and automatically takes into account the umklapp processes exactly. Although the difficulties seem to have been transferred to the determination of the structure factor itself, this is not the case, because the structure factor can be obtained from independent empirical data if necessary (Sec. III).

In Sec. IV, a very simple model for the structure factor of solid metals is proposed which allows us to apply the theory to solid sodium and potassium. The results are compared with available experimental data. The effects of the electron-electron interaction and the approximations involved in the theory are discussed in Sec. V. In the Appendix, it is shown that this theory coincides with Yafet's within the one-phonon approximation.

II. RELAXATION TIME

Following Asik, Ball, and Slichter[11] the spin-relaxation rate is given by

$$\frac{1}{T_1} = -2\sum_{\vec{k}}\sum_{\vec{k}'} \frac{g_{\downarrow}(\vec{k}')[1-g_{\uparrow}(\vec{k})]\,W_{\vec{k}'\downarrow,\vec{k}\uparrow} - g_{\uparrow}(\vec{k})[1-g_{\downarrow}(\vec{k}')]\,W_{\vec{k}\uparrow,\vec{k}'\downarrow}}{\rho'(E_F)\Delta E}\ , \qquad (1)$$

where

$$g_{\uparrow,\downarrow}(\vec{k}) = (e^{\beta(E_k - E_{\uparrow,\downarrow})} + 1)^{-1} \tag{2}$$

are distribution functions for electrons with spin up (↑) and down (↓), $E_{\uparrow,\downarrow} = E_F \pm \frac{1}{2}\Delta E$ and $\beta = (k_B T)^{-1}$, $\rho'(E_F) = m_b k_F/(2\pi^2)$ is the density of states of a given spin direction at the equilibrium Fermi energy E_F calculated using the band effective mass m_b. The transition rate $W_{\vec{k}\uparrow,\vec{k}'\downarrow}$ for spin-flip scattering from the electronic state $|\vec{k},\uparrow)$ to $|\vec{k}',\downarrow)$, with energies E_k and $E_{k'}$, respectively, is given in the first Born approximation by[12]

$$W_{\vec{k}\uparrow,\vec{k}'\downarrow} = 2\pi \sum_n \sum_m p_n \left| \langle n | (\vec{k}',\downarrow | H_{so} | \vec{k},\uparrow) | m \rangle \right|^2 \times \delta(\omega - E_m + E_n), \tag{3}$$

where H_{so} is the spin-orbit Hamiltonian and $\omega = E_k - E_{k'}$. $|m\rangle$ and E_m are the eigenstates and eigenvalues of the lattice, respectively. We use the word *lattice* to denote the ionic system in either the solid or liquid state. The adiabatic approximation is used to separate the electronic and ionic variables. Since we are interested in the electronic spin-flip transition rate only, a sum over all final lattice states $|m\rangle$ and initial states $|n\rangle$ weighted by the probability p_n of finding the lattice in the state $|n\rangle$ is performed.

The matrix element $(\vec{k},\uparrow | H_{so} | \vec{k}',\downarrow)$ has been calculated in Ref. 1. We briefly indicate the model used and the result obtained:

$$H_{so} = \frac{1}{2m^2c^2}\, \vec{s} \cdot \operatorname{grad} V \times \vec{p}\ ; \tag{4}$$

$\vec{s}$ and $\vec{p}$ are the electron-spin and momentum operators, respectively.

The lattice potential V is approximated by a sum of spherically symmetric nonoverlapping potentials v due to ions at positions $\vec{R}_j$,

$$V = \sum_j v(\vec{r} - \vec{R}_j). \tag{5}$$

Then, the spin-orbit interaction becomes

$$H_{so} = \sum_j \xi(\vec{r} - \vec{R}_j)\, \vec{s} \cdot \vec{L}_j, \tag{6}$$

where

$$\xi(r) = \frac{1}{2m^2c^2}\, \frac{1}{r}\, \frac{dv}{dr} \tag{7}$$

and $\vec{L}_j = (\vec{r} - \vec{R}_j) \times \vec{p}$ is the angular-momentum operator referred to the site $\vec{R}_j$. The conduction-electron wave functions are approximated by single orthogonalized plane waves (OPW),

$$|\vec{k}, s) = C_k^{-1/2} \left(|\vec{k}, s\rangle - \sum_{j,\gamma} \langle j,\gamma | \vec{k}, s\rangle\, | j,\gamma\rangle \right). \tag{8}$$

$|\vec{k}, s\rangle$ denotes a plane wave with momentum $\vec{k}$ and spin component s. $|j,\gamma\rangle$ is the core state with quantum numbers n, l, m, s (represented by γ) belonging to the ion at the site $\vec{R}_j$. C_k is a normalization factor.

The matrix element $(\vec{k}',\downarrow | H_{so} | \vec{k},\uparrow)$ has the form

$$(\vec{k}',\downarrow | H_{so} | \vec{k},\uparrow) = \Gamma_{\vec{k}\uparrow,\vec{k}'\downarrow} \sum_j e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_j}. \tag{9}$$

The explicit expression for $\Gamma_{\vec{k}\uparrow,\vec{k}'\downarrow}$ is given in Eq. (29) of Ref. 1. Replacing (9) in (3) and noting that $\Gamma_{\vec{k}\uparrow,\vec{k}'\downarrow}$ does not depend on the ionic coordinates, we have

$$W_{\vec{k}\uparrow,\vec{k}'\downarrow} = 2\pi \left| \Gamma_{\vec{k}\uparrow,\vec{k}'\downarrow} \right|^2 \sum_{n,m} p_n \times \left| \langle n | \sum_j e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_j} | m \rangle \right|^2 \delta(\omega - E_m + E_n)$$

or

$$W_{\vec{k}\uparrow,\vec{k}'\downarrow} = 2\pi \left| \Gamma_{\vec{k}\uparrow,\vec{k}'\downarrow} \right|^2 S(\vec{q},\omega), \tag{10}$$

with $\vec{q} = \vec{k} - \vec{k}'$. $S(\vec{q},\omega)$ is the dynamical-structure factor defined by Van Hove.[13] Substituting for $W_{\vec{k}\uparrow,\vec{k}'\downarrow}$ and $W_{\vec{k}'\downarrow,\vec{k}\uparrow}$ in Eq. (1), we obtain

$$\frac{1}{T_1} = \frac{4\pi}{\Delta E\, \rho'(E_F)} \sum_{\vec{k}} \sum_{\vec{k}'} \Big\{ \left| \Gamma_{\vec{k}\uparrow,\vec{k}'\downarrow} \right|^2 \times S(\vec{q},\omega) g_\uparrow(\vec{k}) [1 - g_\downarrow(\vec{k}')] - \left| \Gamma_{\vec{k}'\downarrow,\vec{k}\uparrow} \right|^2 \times S(-\vec{q},-\omega)\, g_\downarrow(\vec{k}'\rangle [1 - g_\uparrow(\vec{k})] \Big\}. \tag{11}$$

Noting that

$$\left| \Gamma_{\vec{k}\uparrow,\vec{k}'\downarrow} \right|^2 = \left| \Gamma_{\vec{k}'\downarrow,\vec{k}\uparrow} \right|^2$$

and[14]

$$S(-\vec{q},-\omega) = e^{-\beta\omega} S(\vec{q},\omega)$$

and replacing the sums over $\vec{k}$ by integrals using the substitution

$$\sum_{\vec{k}} \to \int \frac{d^3k}{(2\pi)^3} \to \int \rho'(E_k)\, dE_k \frac{d\Omega_k}{4\pi}\ ,$$

Eq. (11) can be written as

$$\frac{1}{T_1} = \frac{4\pi}{\Delta E \rho'(E_F)} \int \left| \Gamma_{\vec{k}\uparrow,\vec{k}'\downarrow} \right|^2 S(\vec{q},\omega) \times \left\{ g_\uparrow(E)[1 - g_\downarrow(E')] - g_\downarrow(E')[1 - g_\uparrow(E)]\, e^{\beta(E'-E)} \right\} \times \frac{\rho'(E)\, \rho'(E') dE\, dE'\, d\Omega\, d\Omega'}{(4\pi)^2}, \tag{12}$$

where E and E' stand for E_k and $E_{k'}$, respectively. Developing the functions $g_{\uparrow,\downarrow}$ up to first order in ΔE, we find

$$g_{\uparrow,\downarrow}(E) = g_0(E) \pm \tfrac{1}{2}\beta\Delta E\, g_0(E)\, [1 - g_0(E)],$$

where $g_0(E) = (e^{\beta(E - E_F)} + 1)^{-1}$. Using the identity

$$g_0(E)\,[1-g_0(E')]=g_0(E')\,[1-g_0(E)]\,e^{\beta(E'-E)}\,,$$

Eq. (12) can be rearranged as

$$\frac{1}{T_1}=\frac{4\pi\beta}{\rho'(E_F)}\int |\Gamma_{\vec{k}',\vec{k}'_\downarrow}|^2\, S(\vec{q},\omega)\, g_0(E)\,[1-g_0(E')] \times\frac{\rho'(E)\,\rho'(E')\,dE\,dE'\,d\Omega\, d\Omega'}{(4\pi)^2}\,. \tag{13}$$

Handling the energy integrals like GK,[3] Eq. (13) reduces to

$$\frac{1}{T_1}=\frac{m_b k_F}{(2\pi)^3}\int d\Omega\, d\Omega'\, |\Gamma_{\vec{k}_F',\vec{k}'_{F\downarrow}}|^2\, S(\vec{q}), \tag{14}$$

with[15]

$$S(\vec{q})=\int_{-\infty}^{\infty} d\omega\, \frac{\beta\omega}{e^{\beta\omega}-1}\, S(\vec{q},\omega). \tag{15}$$

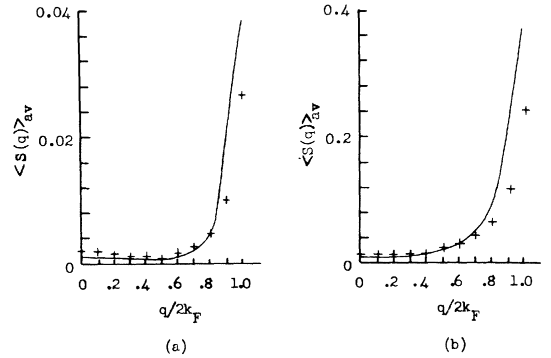
Equation (14) simplifies considerably if $S(\vec{q})$ depends only on the modulus q. This is the case for liquid metals. Then, three angular integrals can be performed analytically leaving the remaining one, that in q, to be calculated numerically. The result, hereafter called "reduced Eq. (14)," is given by Eq. (19) of Ref. 6 with $c_\mu=1$, $c_\nu=0$ for $\nu\neq\mu$ (corresponding to a single-component substance instead of an alloy).

III. STRUCTURE FACTOR

Equation (14) can be used to calculate the spin-lattice relaxation rate in a metal in both the solid and liquid states.[16] In liquid metals the range of values of ω which give a relevant contribution to the integral (15) is such that $\beta|\omega|\ll 1$. Hence, to a good approximation $S(q)$ can be replaced by the static-structure factor

$$S(q)=\int_{-\infty}^{\infty} d\omega\, S(q,\omega). \tag{16}$$

$S(q)$ can be obtained empirically from slow-neutron–[17] or x-ray–[18] scattering experiments or, theoretically, using a model for the liquid metal.[19] In simple liquid metals, it is a good approximation to put $m_b=m$.



(a) (b)

FIG. 1. Average structure factor. Solid line, Greene and Kohn; crosses, simple model: (a) at 40 °K, (b) at 273 °K.

For solid metals, owing to the lack of direct empirical information about $S(\vec{q},\omega)$ we follow GK in writing the structure factor in the one-phonon approximation,

$$S(\vec{q})=\frac{\beta}{MN}\sum_p \frac{(\vec{\xi}_p\cdot\vec{q})^2}{(e^{\beta\omega_{\vec{q}p}}-1)(1-e^{-\beta\omega_{\vec{q}p}})}\,, \tag{17}$$

and averaging over all directions of $\vec{q}$:

$$\langle S(\vec{q})\rangle_{\text{av}}=\int\frac{d\Omega_q}{4\pi}\, S(\vec{q}). \tag{18}$$

Here M is the ionic mass, N the ionic density, and $\omega_{\vec{q}p}$ the dispersion of a phonon with polarization unit vector $\vec{\xi}_p$. The sum runs over the phonon branches denoted by the index p (= 1, 2, 3).

The approximation of $S(\vec{q})$ by the isotropic-structure factor $\langle S(\vec{q})\rangle_{\text{av}}$ allows the use of the reduced expression for T_1^{-1}. Detailed resistivity calculations in sodium,[3] where this approximation is checked, suggest that the error introduced is negligible.

$\langle S(\vec{q})\rangle_{\text{av}}$ can be computed on the basis of empirical phonon dispersion curves, and although the procedure does not involve any difficulty, it is rather cumbersome.

IV. APPLICATION

As a first approach to assess the adequacy of this theory we use a very simple model for the structure factor of a solid. It is assumed that the three acoustical-phonon branches have the same spherically symmetric dispersion ω_q. Hence,

$$\langle S(\vec{q})\rangle_{\text{av}}=(q^2\beta/2MN)[\cosh(\beta\omega_q)-1)]^{-1}. \tag{19}$$

We use the phonon dispersion given by the Born–von Kármán model,[20]

$$\omega_q=(2vq_D/\pi)\,|\sin(\pi q/2q_D)|\ . \tag{20}$$

Here v is some average sound velocity which can be chosen as $v=(NMX)^{-1/2}$, where X is the isothermal compressibility, so that $\langle S(\vec{q})\rangle_{\text{av}}$ has the correct limit $\langle S(0)\rangle_{\text{av}}=k_BTX$.[21] In the calculations we use simply $v=v_l$ (longitudinal sound velocity) which may lead to underestimate $\langle S(\vec{q})\rangle_{\text{av}}$ for large q since $v_l>(NMX)^{-1/2}$. q_D is the radius of the Debye sphere. For the alkali metals, with body-centered cubic structure, q_D is obtained from

$$\tfrac{4}{3}\pi q_D^3=\tfrac{1}{4}(4\pi/a)^3, \tag{21}$$

where a is the lattice constant. Using these simplifications, the structure factors for sodium and potassium in the temperature range 300–10 °K have been calculated. {*Note added in proof.* The longitudinal sound velocity was calculated from $v_l=(c_{11}/\rho)^{1/2}$. The temperature-dependent elastic

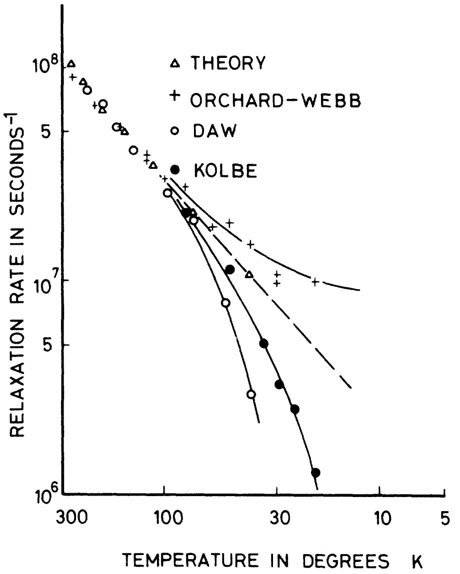


FIG. 2. Relaxation rate in sodium.

constant $c_{11}(T)$ was taken from M. E. Diederich and J. Trivisino [J. Phys. Chem. Solids 27, 637 (1966)] and W. R. Marquardt and J. Trivisino [J. Phys. Chem. Solids 26, 273 (1965)] for sodium and potassium, respectively. The values of $c_{11}(T)$ for $T < 77$°K were obtained by linear extrapolation. The density $\rho(T)$ was taken from W. B. Pearson [*Handbook of Lattice Spacings and Structures of Metals and Alloys* (Pergammon, New York, 1958)]}. In order to estimate the errors introduced by these approximations we have compared our results for sodium at 40 and 273 °K with those of GK (Fig. 1). Considering the large interval between these two temperatures the agreement is not bad. Errors of the order of 50% in T_1 can be expected, however. This is estimated comparing T_1^{-1} at 40 and 273 °K calculated using the GK structure factors, which give 1.1×10^7 and 1.4×10^8 sec^{-1}, respectively,[2] with our results, 1.1×10^7 and 1.0×10^8 sec^{-1}, respectively.

With this model for the structure factor, the spin-relaxation rate in sodium and potassium has been calculated as a function of temperature using the reduced Eq. (14). The radial-core wave functions and the self-consistent potential of the ions in the metal were approximated by those of the free atom,[22] with an estimated error of less than 1%. Figure 2 shows the results for sodium; the experimental data are of Daw,[9] Kolbe,[10] and Orchard-Webb.[23] Figure 3 shows the results for potassium together with the experimental data reported by Walsh, Rupp, and Schmidt.[24] Good agreement is found for both metals down to about 40 °K. The possible origin of the discrepancies occurring below 40 °K are discussed in Sec. V.

In calculations we have assumed that m_b equals the free-electron mass; this appears to be justifiable for both sodium and potassium.[11,25]

V. DISCUSSION

The SRT given by Eq. (14) has to be corrected for the effects of electron-electron interactions,[26]

$$T_1^{\rm eff} = T_1/\kappa_0^2 \,. \tag{22}$$

The exchange-enhancement factor $\kappa_0^2 \leq 1$ is related to the electron-electron interaction parameter B_0 and the quasiparticle mass m^* by

$$\kappa_0^{-2} = \frac{m^*/m}{1+B_0} \,, \tag{23}$$

where the quasiparticle mass includes band-structure effects, phonon effects, and electron-electron interaction effects.

B_0 equals -0.215 ± 0.03 and -0.285 ± 0.02 for sodium and potassium, respectively,[27] while m^*/m has the values 1.24 ± 0.02 and 1.21 ± 0.02.[28] Hence, κ_0^{-2} amounts to 1.58 ± 0.08 and 1.69 ± 0.07 for sodium and potassium, respectively. The measured SRT T_{1m} must be identified with $T_1^{\rm eff}$.

Phonon corrections to B_0 and m^* cancel each other in Eq. (23). Hence, if band-structure corrections to the free-electron model are negligible, as in the cases of Na and K, the values of κ_0^{-2} given by (23) are valid for both the solid and liquid

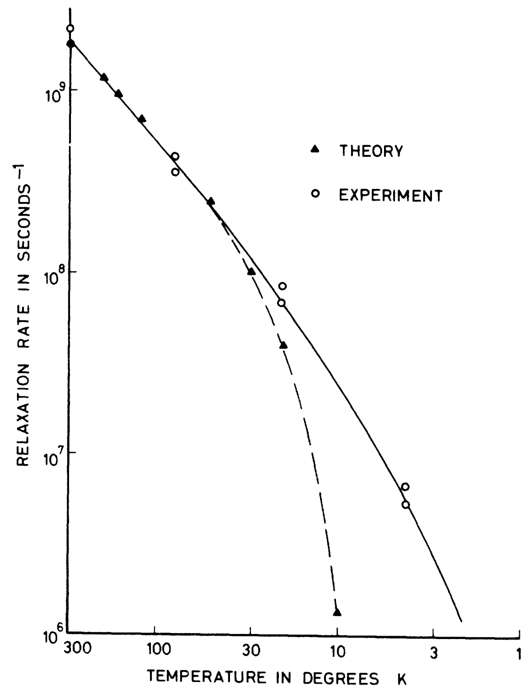


FIG. 3. Relaxation rate in potassium. [Experimental values of Walsh, Rupp, and Schmidt (Ref. 24)].

states.[29] The values of κ_0^{-2} estimated from the relation T_{1m}/T_1 for liquid sodium and potassium are 1.58 ± 0.30 and 1.93 ± 0.50, respectively.[7]

The crudeness of the model used here to calculate the structure factors does not allow the determination of meaningful values of κ_0^{-2} for solid Na and K from the relation T_{1m}/T_1. In fact, the almost perfect agreement between T_1 and the measured relaxation rates down to 40 °K shown in Figs. 2 and 3 must be considered rather coincidental since errors of the order of 50% in T_1 can be expected. With the values of T_1 at 40 and 273 °K obtained using the GK structure factors for Na (9.0×10^{-8} and 7.3×10^{-9} sec, respectively[2]), T_{1m}/T equals 1.78 and 1.5, respectively, which within the errors is consistent with the theoretical value (1.58 ± 0.08) and the experimental value obtained for liquid Na (1.58 ± 0.3).[7]

The use of single OPW to approximate the conduction-electron wave functions may lead to overestimate the SRT. Rough estimates indicate that the error should be negligible for Na but it may start to be important for potassium.[6]

The theory has been found to predict well the temperature dependence of the spin-relaxation rate at least down to 40 °K for both sodium and potassium. The discrepancy found in the case of sodium below that temperature could be attributed to the phase transition from body-centered cubic to hexagonal close-packed structure that occurs around 36 °K and which has not been taken into account in the theory.

The cause of the discrepancy in potassium could be the presence of small amounts of impurities in the experimental samples which would contribute to the spin-relaxation rate with a temperature-independent term. A high concentration of impurities makes the relaxation rate tend to a constant value at relatively high temperatures (this seems to be the case with Orchard-Webb's results for sodium[23]).

At very low temperatures other relaxation mechanisms than spin-orbit scattering may become important, particularly the spin-current interaction.[30] However, a simple calculation shows that for both sodium and potassium the magnitude of its contribution to the relaxation is negligible in the temperature range considered here.

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APPENDIX: COMPARISON WITH YAFET'S THEORY

The system is described by the Hamiltonian

$$H = H_e + V' + H'_{so} + \delta V' + \delta H'_{so}, \tag{A1}$$

where H_e is the free-electron Hamiltonian, V' the perfect-lattice potential, H'_{so} the spin-perfect-lattice interaction, $\delta V'$ the perturbation of the lattice potential due to phonons, and $\delta H'_{so}$ the perturbation of the spin-lattice interaction due to phonons.

That part of the spin-orbit interaction which does not induce spin-flip transitions is supposed to be included in the lattice potential.

We call $\varphi_{\vec{k},s}$ the eigenfunctions of the Hamiltonian $H_0 = H_e + V'$; these are Bloch functions with definite spin component s (up or down). $E_{\vec{k}}$ are the corresponding eigenvalues.

Yafet considers the "unperturbed" Hamiltonian $H_0 + H'_{so}$. Up to first order in H'_{so} its eigenfunctions, in terms of the $\varphi_{\vec{k},s}$, are given by

$$\psi_{\vec{k}\uparrow} = \varphi_{\vec{k}\uparrow} + \sum_{\vec{k}''} \frac{\langle \varphi_{\vec{k}''\downarrow} | H'_{so} | \varphi_{\vec{k}\uparrow} \rangle}{E_{\vec{k}} - E_{\vec{k}''}} \varphi_{\vec{k}''\downarrow}, \tag{A2}$$

and analogously for spin down. The spin-flip matrix element calculated by Yafet is

$$M_Y = \langle \psi_{\vec{k}'\downarrow} | \delta V' + \delta H'_{so} | \psi_{\vec{k}\uparrow} \rangle = \langle \varphi_{\vec{k}'\downarrow} | \delta H'_{so} | \varphi_{\vec{k}\uparrow} \rangle$$

$$+ \sum_{\vec{k}''} \frac{\langle \varphi_{\vec{k}'\downarrow} | \delta V' | \varphi_{\vec{k}''\downarrow} \rangle \langle \varphi_{\vec{k}''\downarrow} | H'_{so} | \varphi_{\vec{k}\uparrow} \rangle}{E_{\vec{k}} - E_{\vec{k}''}} + \sum_{\vec{k}''} \frac{\langle \varphi_{\vec{k}'\downarrow} | H'_{so} | \varphi_{\vec{k}''\uparrow} \rangle \langle \varphi_{\vec{k}''\uparrow} | \delta V' | \varphi_{\vec{k}\uparrow} \rangle}{E_{\vec{k}'} - E_{\vec{k}''}} + O(H'^2_{so}\,\delta H'_{so}). \tag{A3}$$

In this work the "unperturbed" Hamiltonian $H_0 + \delta V'$ is considered. Its eigenfunctions, which contain the ionic position operators $\vec{R}_j$ through $\delta V'$, can also be written in terms of the $\varphi_{\vec{k}s}$. Up to first order in $\delta V'$ they are

$$\Phi_{\vec{k}\uparrow} = \varphi_{\vec{k}\uparrow} + \sum_{\vec{k}''} \frac{\langle \varphi_{\vec{k}''\uparrow} | \delta V' | \varphi_{\vec{k}\uparrow} \rangle}{E_{\vec{k}} - E_{\vec{k}''}} \varphi_{\vec{k}''\uparrow}, \tag{A4}$$

and analogously for spin down. It is assumed that the electron wave function follows the ionic motion adiabatically. It should be noted that in this paper the functions $\Phi_{\vec{k}s}$ are approximated by single OPW, that is by plane waves orthogonalized to the core states of each ion at its position $\vec{R}_j$. The spin-flip matrix element used in this work is

$$M_{\mathrm{DH}} = \langle \Phi_{\vec{k}'\downarrow} | H'_{so} + \delta H'_{so} | \Phi_{\vec{k}\uparrow} \rangle = \langle \varphi_{\vec{k}'\downarrow} | H'_{so} | \varphi_{\vec{k}\uparrow} \rangle + \langle \varphi_{\vec{k}'\downarrow} | \delta H'_{so} | \varphi_{\vec{k}\uparrow} \rangle + \sum_{\vec{k}''} \frac{\langle \varphi_{\vec{k}'\downarrow} | H'_{so} | \varphi_{\vec{k}''\uparrow} \rangle \langle \varphi_{\vec{k}''\uparrow} | \delta V' | \varphi_{\vec{k}\uparrow} \rangle}{E_{\vec{k}} - E_{\vec{k}''}}$$

$$+ \sum_{\vec{k}''} \frac{\langle \varphi_{\vec{k}'\downarrow} | \delta V' | \varphi_{\vec{k}''\downarrow} \rangle \langle \varphi_{\vec{k}''\downarrow} | H'_{so} | \varphi_{\vec{k}\uparrow} \rangle}{E_{\vec{k}'} - E_{\vec{k}''}} + O(\delta V' \delta H'_{so}) + O[(\delta V')^2 H'_{so}]. \tag{A5}$$

In the calculation of the SRT only those transitions for which $E_{\vec{k}} = E_{\vec{k}'} = E_F$ need to be considered. In this case $\langle \varphi_{\vec{k}'_F\downarrow} | H'_{so} | \varphi_{\vec{k}_F\uparrow} \rangle$ vanishes because H'_{so} only links states belonging to different bands, and the expressions (A3) and (A5) become identical up to first order in the spin-orbit interaction and within the one-phonon approximation

$$M_Y(E_{\vec{k}} = E_{\vec{k}'}) = M_{DH}(E_{\vec{k}} = E_{\vec{k}'}) + O[H'^2_{so} \delta H'_{so},\ \delta V' \delta H'_{so},\ (\delta V')^2 H_{so}]. \tag{A6}$$

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[15] Equation (15) for $S(\vec{q})$ reduces to that of GK using their definition of the dynamical-structure factor: $S_{\mathrm{GK}}(\vec{q}, \omega) = S(-\vec{q}, -\omega)$.

[16] The application to solids of Eq. (14) with (18) was first proposed in Ref. 2.

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