Supplementary information A unified theory of spin-relaxation due to spin-orbit coupling in metals and semiconductors

Péter Boross,^{1,2} Balázs Dóra,^{1,3} Annamária Kiss,^{1,4} and Ferenc Simon^{1,5, *}

¹Department of Physics, Budapest University of Technology and Economics, Budapest, Hungary

²Department of Materials Physics, Eötvös University, Budapest, Hungary

³BME-MTA Exotic Quantum Phases Research Group, Budapest University of Technology and Economics, Budapest, Hungary

⁴Wigner Research Centre for Physics of the Hungarian Academy of Sciences, Budapest, Hungary

⁵Condensed Matter Physics Research Group of the Hungarian Academy of Sciences, Budapest, Hungary

This Supplementary Material is organized as follows: we discuss the generalization of the spin-relaxation for two kinds of band dispersions (quadratic and linear or linearized) when the restrictions concerning the relative magnitude of the parameters (∆*, µ, m[∗]*) are lifted. We arrive at the overall conclusion that while the quantitative details of the Γ dependent spin-relaxation (Γ_s) are modified and no closed form of the result can be provided in the most general case, the overall trends, which characterize the EY and DP behaviors and in particular the crossover between the two, remain valid. Wherever possible, we provide closed form results though. Finally, we discuss the spin-relaxation for a model where only Rashba-type spin-relaxation is present.

I. SPIN-RELAXATION FOR DIFFERENT MODEL DISPERSIONS

A. Quadratic dispersion model

First, we discuss a quadratic model with the $\epsilon_{k,\alpha} = \hbar^2 k^2 / 2m_\alpha^* - \delta_{\alpha,1}\Delta$ single-particle dispersion. In the conduction band, the quasi-particles are electron-type (i.e. $m_2^* > 0$) however the quasi-particles of a nearby band are hole-type (i.e. $m_2^* < 0$). The band structure is depicted in Fig. 1. This model describes well two bands of the spectrum of semiconductors, however in a realistic case (e.g. for Si and GaAS) there are more nearby bands characterized by different band gaps and effective masses.

1. The intra-band term

An important and general limit of the model is when the Zeemann energy is much smaller than the band gap (i.e. $\Delta_Z \ll \Delta$), and both the spin-up and spin-down states are occupied in the conduction band (i.e. Δ _Z $\ll \mu$). In this limit, the intra-band term

FIG. 1: Band structure of quadratic dispersion model. Vertical arrows show the energy separations between the relevant bands.

can be expressed as

$$
\Gamma_{\rm s}^{\rm intra} = \frac{4\left|\mathcal{L}\left(k_{\rm F}\right)\right|^2 \Gamma}{4\Gamma^2 + \Delta_Z^2}.\tag{1}
$$

This term comes from processes within the conduction band and the nearby band does not give a contribution to the intra-band term.

2. The inter-band term in the general case

In the Δ _Z $\ll \mu$, Δ limit, the inter-band term can be determined but it takes a more complicated form. When the broadening is much smaller than the energy separation at the Fermi wavenumber (i.e. $\Gamma \ll \Delta (k_F) = \Delta + (1 - m_2^*/m_1^*) \mu$) the inter-band spin-relaxation has the form of

$$
\Gamma_{\rm s}^{\rm inter} = \frac{4 \left| L \left(k_{\rm F} \right) \right|^2}{\Delta^2 \left(k_{\rm F} \right)} \Gamma, \tag{2}
$$

which is directly proportional to the momentum-scattering rate.

When the broadening is much larger than the energy separation (i.e. $\Gamma \gg \Delta (k_F)$) the spin-relaxation reads

$$
\Gamma_{\rm s}^{\rm inter} = \frac{-4m_1^*m_2^*|L(k_{\rm F})|^2}{\left(m_2^*-m_1^*\right)^2} \frac{1}{\Gamma},\tag{3}
$$

which is inversely proportional to the momentum-scattering rate.

3. The inter-band term in the case of $m_1^* = -m_2^*$

If the effective masses in the two bands have different signs but the same magnitude, the spin-relaxation rate is obtained as

$$
\Gamma_{\rm s}^{\rm inter} = \frac{4 \left| L \left(k_{\rm F} \right) \right|^2 \Gamma}{4 \Gamma^2 + \Delta^2 \left(k_{\rm F} \right)} \left[1 + \frac{\Gamma \ln \frac{\Gamma^2 + \mu^2}{\Gamma^2 + (\Delta + \mu)^2}}{\left(\Delta + 2\mu \right) \left(\pi + \arctan \frac{\mu}{\Gamma} - \arctan \frac{\Delta + \mu}{\Gamma} \right)} \right]. \tag{4}
$$

4. The inter-band term in the case of $m_1^* = -m_2^*$ *and* $\mu \gtrsim \Delta$

When the Fermi energy is not close to the bottom of the conduction band, the logarithmic term can be neglected and we obtain the most compact form of the inter-band spin-relaxation rate as

$$
\Gamma_{\rm s}^{\rm inter} = \frac{4 \left| L \left(k_{\rm F} \right) \right|^2 \Gamma}{4 \Gamma^2 + \Delta^2 \left(k_{\rm F} \right)}.
$$
\n
$$
\tag{5}
$$

5. Summary of the result for the quadratic model

Summing of intra- and inter-band term yields Eq. (15) of the paper:

$$
\Gamma_{\rm s} = \frac{4\left|\mathscr{L}\left(k_{\rm F}\right)\right|^2 \Gamma}{4\Gamma^2 + \Delta_Z^2} + \frac{4\left|L\left(k_{\rm F}\right)\right|^2 \Gamma}{4\Gamma^2 + \Delta^2 \left(k_{\rm F}\right)}.\tag{6}
$$

This is the main result, which is presented in the manuscript.

We note that similar expressions can be obtained if the chemical potential lies in the nearby band.

FIG. 2: Linear band dispersion models, with line slopes of the opposite (a) and the same sign (b). The first situation can be obtained e.g. from linearizing a quadratic band dispersion in Fig. 1 and the second occurs e.g. for MgB_2 as shown in Ref. 1.

B. Linear band dispersion models

Herein, we discuss the spin-relaxation time for linear model dispersions. The importance of studying this model is two-fold. First, every non-linear band dispersions can be linearized at the Fermi wave-vector and the plausible expectation is that the spin-relaxation rate can be obtained as a sum of the linearized segments. Second, spin-relaxation can be calculated for the linear band dispersion model and as we show below, the qualitative result, i.e. dependence of Γ_s on Γ for the intra- and inter-band processes, is unchanged compared to the quadratic band dispersion even if the numerical factors are different. This proves that our calculation of the spin-relaxation is robust against the details of the band dispersion.

The linear band-dispersion models can take two characteristically different scenarios: those with lines with slopes of the opposite and the same sign. The situation is depicted in Fig. 2. The first situation can be obtained e.g. from linearizing a quadratic band dispersion in Fig. 1 the Fermi wavenumber and the second occurs e.g. for MgB_2 as shown in Ref. [1].

1. Linear band dispersions with the opposite slope

We consider that the higher lying conduction band has a positive Fermi velocity thus $\epsilon_{k,2}^{\text{lin}} = \hbar v_2^{\text{F}}(k - k_{\text{F}}) + \mu$, where the Zeeman-energy is neglected. The nearby valence band can be approximated with a flat band with zero Fermi velocity: $\epsilon_{k,1}^{\text{lin}} =$ $-\Delta + \mu m_2^* / m_1^*$, where the Zeeman splitting is also neglected too.

Then, our calculation yields for the intra-band contribution to the spin-relaxation rate:

$$
\Gamma_{\rm s}^{\rm intra} = \frac{4\Gamma \left| \mathcal{L}\left(k_{\rm F}\right) \right|^2}{4\Gamma^2 + \Delta_Z^2}.\tag{7}
$$

Similarly, we obtain for the inter-band term:

$$
\Gamma_{\rm s}^{\rm inter} = \frac{4 \left| L \left(k_{\rm F} \right) \right|^2 \Gamma}{\Gamma^2 + \Delta^2 \left(k_{\rm F} \right)},\tag{8}
$$

which look likes as if it was obtained from the quadratic model Eq. (5) except the multiplication factor of the Γ^2 in the denominator. This is the result that we considered a zero Fermi velocity of the valence band.

2. Linear band dispersions with the same slope

The second linear model has two linear bands (apart from the spin) with positive Fermi velocities of different magnitudes. The two bands cross the Fermi level at two separate points. The band structure of this model is depicted in Fig. 2b. This model describes the spectrum around the Fermi energy in e.g. $MgB₂$ as it was shown in Ref. 1.

The intra-band term is similar to the previous results and it reads:

$$
\Gamma_s^{\text{intra}} = \frac{4\Gamma \left| \mathcal{L}\left(k_{\text{F}}\right) \right|^2}{4\Gamma^2 + \Delta_Z^2}.
$$
\n(9)

The inter-band term can be expressed as

$$
\Gamma_s^{\text{inter}} = \frac{4\Gamma \left| L \left(k_{\text{F}} \right) \right|^2}{\frac{\left(\Delta_1 + \Delta_2 \right)^2}{\Delta_1 \Delta_2} \Gamma^2 + \Delta_1 \Delta_2},\tag{10}
$$

where Δ_1 and Δ_2 are the distances of the two bands when one of the bands cross the Fermi level. The formula is symmetric in these two variables which means that the two bands change their roles as conduction and valence bands for the two Fermi level crossing points.

A special case is when $v_1^{\text{F}} = v_2^{\text{F}}$, i.e. when the two linear bands are parallel therefore $\Delta_1 = \Delta_2 = \Delta$. This yields a result which is similar to the case of the quadratic dispersion and reads:

$$
\Gamma_{\rm s}^{\rm inter} = \frac{4\Gamma \left| L \left(k_{\rm F} \right) \right|^2}{4\Gamma^2 + \Delta^2}.
$$
\n(11)

II. THE SPIN-RELAXATON FOR A MODEL WITH RASHBA-LIKE SOC

Now we determine the spin-relaxation rate of a model where only Rashba-type SOC is present. The Rashba-like SOC can be written as

$$
\mathcal{H}_{\text{SO}} = \sum_{k,\alpha} \hbar \lambda \left(\sigma_x k_y - \sigma_y k_x \right),\tag{12}
$$

where σ_x , σ_y are the Pauli matrices. The matrix element of intra-band SOC can be expressed as $|\mathscr{L}(k)| = \hbar \lambda k$. We can expand Eq. (6) to get

$$
\Gamma_{\rm s} = \frac{8m_2^* \mu \lambda^2}{4\Gamma^2 + \Delta_Z^2}.\tag{13}
$$

Using the spin and momentum life-times instead of relaxation-rates, we obtain

$$
\frac{1}{\tau_{\rm s}} = \frac{8m_2^*\mu\lambda^2}{\hbar^2} \frac{\tau}{1 + \left(\frac{\Delta z\tau}{\hbar}\right)^2}.
$$
\n(14)

A similar expression was obtained recently (Eq. (40) in [2]) for this particular case.

[∗] Electronic address: simon@esr.phy.bme.hu

^[1] F. Simon, B. Dóra, F. Murányi, A. Jánossy, S. Garaj, L. Forró, S. Bud'ko, C. Petrovic, and P. C. Canfield, Phys. Rev. Lett. 101, 177003 (2008).

^[2] A. A. Burkov and L. Balents, Phys. Rev. B 69, 245312 (2004).