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## Semiconductor spintronics in a participating phonon medium: Macroscopic equations

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In the last two decades considerable interest has arisen on the spin related phenomena in semiconductor devices. In semiconductor materials two essential mechanisms act on the spin dynamics: the spin-orbit coupling and the spin-flip interactions. Here the novelty is that we adopt the asymptotic approach developed in previous papers of mine [A. Rossani, *Physica A* **305**, 323 (2002); A. Rossani, G. Spiga, and A. Domaingo, *J. Phys. A* **36**, 11955 (2003); A. Rossani and G. Spiga, *J. Math. Phys.* **47**, 013301 (2006); A. Rossani and A. M. Scarfone, *Physica B* **334**, 292 (2003); A. Rossani, *J. Phys. A* **43**, 165002 (2010)]. The aim of this paper is to derive macroscopic equations starting from a kinetic approach. Moreover an equation for the evolution of the spin density is added, which account for a general dispersion relation. The treatment of spin-flip processes, derived from first principles, is new and leads to an explicit expression of the relaxation time as a function of the temperature. © 2013 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution 3.0 Unported License. [<http://dx.doi.org/10.1063/1.4822161>]

### I. INTRODUCTION

In the last two decades considerable interest has arisen on the spin related phenomena in semiconductor devices. In semiconductor materials two essential mechanisms act on the spin dynamics: the spin-orbit coupling and the spin-flip interactions. The spin-orbit coupling manifests itself by an effective magnetic field seen by the electron which causes the spin precession around it. The Rashba spin-orbit coupling is proportional to the external electric field. Otherwise, the so-called Dresselhaus one arises from the asymmetry present in certain crystal lattices.

The spin-flip processes are interactions between the particles and the crystal with reversal of the spin direction (Elliot-Yafet mechanism). The ensemble of electrons can be described by the Boltzmann spinor equation, which recently has given rise the interest of mathematicians.<sup>4(a),4(b)</sup> In particular, asymptotic expansion techniques have been utilized for the construction of macroscopic equations (see Ref. 2 and references therein). In these models the phonons are considered as a fixed background at a given temperature. Moreover an isotropic parabolic dispersion relation is assumed for electrons.

Here we construct a new asymptotic expansion approach, with the following new features with respect to:<sup>2</sup>

- a) phonons are considered as a participating population<sup>8</sup>
- b) an equation for the evolution of the spin density is constructed where spin flip effects are derived from first principles.
- c) the hypothesis of parabolic dispersion relation for electrons is dropped

In the present paper we start from the (spinor) Bloch-Boltzmann-Peierls (BBP) coupled equations for the distribution functions of electrons and phonons.

After that, by means of an expansion<sup>3</sup> of both the unknowns and the interaction kernels with respect to a small parameter which accounts for the umklapp processes (with no momentum conservation), the lowest order equations show that the displaced Fermi-Dirac (for electrons) and

Bose-Einstein (for phonons) approximation is justified. A closed set of equations for the chemical potential of electrons, the temperature of the mixture, and the drift velocity can be constructed, which recalls the extended thermodynamics model.<sup>1</sup> Moreover, an equation for the time evolution of the spin density is added.

## II. THE SPINOR KINETIC EQUATIONS

Consider two interacting populations: electrons (e), with charge -e, and phonons (p). Let  $N_g(\mathbf{k}, \mathbf{x}, t)$  be the distribution function of phonons [quasi-momentum  $\mathbf{k}$ , energy  $\omega_g(\mathbf{k})$ ] of type  $g$  (i.e. branch  $g$  of the phonon spectrum) and  $F_p = F_p(\mathbf{p}, \mathbf{x}, t)$  the matrix ( $2 \times 2$ ) distribution function of electrons (quasi-momentum  $\mathbf{p}$ , energy  $\mathcal{E}_p$ ). We can write also

$$F_p = (1/2)f_p^c \mathbf{I} + \mathbf{f}_p^s \cdot \vec{S},$$

( $\vec{S}$  are the Pauli's matrices and  $\mathbf{I}$  is the unit  $2 \times 2$  matrix) where we separated the charge (c) and the spin (s) distribution functions.

By neglecting e-e interactions, the BBP equations read

$$\mathcal{D}_g N_g = (\partial N_g / \partial t)_{pp} + (\partial N_g / \partial t)_{pe} + (\partial N_g / \partial t)_{sf}, \quad (1)$$

where p-p, p-e, and sf interactions are accounted for (the sf term is given in the appendix), and

$$\mathcal{D}_p F_p = (\partial F_p / \partial t)_{ep} + (\partial F_p / \partial t)_{so} + (\partial F_p / \partial t)_{sf} \quad (2)$$

where we consider e-p, (so) spin-orbit, and (sf) spin-flip (see again the appendix) interactions. Explicitly

$$\mathcal{D}_g = \partial / \partial t + \mathbf{u}_g \cdot \partial / \partial \mathbf{x}, \quad \text{where } \mathbf{u}_g = \partial \omega_g / \partial \mathbf{k}, \quad (3)$$

$$\mathcal{D}_p = \partial / \partial t + \mathbf{v} \cdot \partial / \partial \mathbf{x} - e\mathbf{E} \cdot \partial / \partial \mathbf{p}, \quad \text{where } \mathbf{v} = \partial \mathcal{E}_p / \partial \mathbf{p} \quad (4)$$

Observe that, since  $\omega_g$  and  $\mathcal{E}_p$  are even,  $\mathbf{u}_g$  and  $\mathbf{v}$  are odd.

At the right hand sides of the BBP equations for phonons<sup>7</sup> we have

$$\begin{aligned} (\partial N_g / \partial t)_{pp} = & \int [(1/2) \sum_{g_1 g_2} w_{pp}(\mathbf{k}_1, \mathbf{k}_2 \rightarrow \mathbf{k}) (-N_g(1 + N_{g_1})(1 + N_{g_2}) + (1 + N_g)N_{g_1}N_{g_2}) \\ & + \sum_{g_1 g_3} w_{pp}(\mathbf{k}, \mathbf{k}_1 \rightarrow \mathbf{k}_3)(1 + N_g)(1 + N_{g_1})N_{g_3} - N_g N_{g_1}(1 + N_{g_3})] d\mathbf{k}_1, \end{aligned}$$

where

$$\mathbf{k}_2 = \mathbf{k} - \mathbf{k}_1 + \mathbf{b}(\mathbf{k}_1, \mathbf{k}_2 \rightarrow \mathbf{k}), \quad \mathbf{k}_3 = \mathbf{k} + \mathbf{k}_1 + \mathbf{b}(\mathbf{k}, \mathbf{k}_1 \rightarrow \mathbf{k}_3)$$

( $\mathbf{b}$  is an appropriate vector belonging to the reciprocal lattice), which account for three-phonon processes:

$$(g, \mathbf{k}) \rightleftharpoons (g_1, \mathbf{k}_1) + (g_2, \mathbf{k}_2), \quad (g_3, \mathbf{k}_3) \rightleftharpoons (g, \mathbf{k}) + (g_1, \mathbf{k}_1).$$

Moreover

$$(\partial N_g / \partial t)_{pe} = \int w_{pe}(\mathbf{p} \rightarrow \mathbf{p}', \mathbf{k})(f_p^c(1 + N_g) - f_{p'}^c N_g) d\mathbf{p},$$

where  $\mathbf{p}' = \mathbf{p} - \mathbf{k} + \mathbf{b}(\mathbf{p} \rightarrow \mathbf{p}', \mathbf{k})$  is the difference between the number of phonons  $\mathbf{k}$  emitted by electrons with any quasimomenta  $\mathbf{p}$  and the number of phonons absorbed by electrons with any  $\mathbf{p}'$ .

For electrons we have

$$\begin{aligned} (\partial F_p / \partial t)_{ep} = & \sum_g \int w_{ep}(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p}) [F_{p'} N_g - F_p (N_g + 1)] \\ & + w_{ep}(\mathbf{p}'' \rightarrow \mathbf{p}, \mathbf{k}) (F_{p''} (1 + N_g) - F_p N_g) d\mathbf{k}, \end{aligned}$$

where

$$\mathbf{p}' = \mathbf{p} - \mathbf{k} + \mathbf{b}(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p}), \quad \mathbf{p}'' = \mathbf{p} + \mathbf{k} + \mathbf{b}(\mathbf{p}'' \rightarrow \mathbf{p}, \mathbf{k}),$$

The first term corresponds to processes with emission of a phonon having quasimomentum  $\mathbf{k}$  by an electron having a given quasimomentum  $\mathbf{p}$  and reverse processes. The second term corresponds to processes with absorption of a phonon by an electron with quasimomentum  $\mathbf{p}$  and reverse processes.

The  $w$ 's are transition probabilities which account for energy conservation and satisfy the following symmetry relations:

$$w_{pe}(\mathbf{p} \rightarrow \mathbf{p}', \mathbf{k}) = w_{ep}(\mathbf{p} \rightarrow \mathbf{p}', \mathbf{k}) = w_{ep}(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p}).$$

The so term is given by

$$(\partial \mathbf{F}_{\mathbf{p}} / \partial t)_{so} = (i/2)[\boldsymbol{\Omega} \cdot \vec{\mathbf{S}}, \mathbf{F}_{\mathbf{p}}],$$

where  $[C, D] = CD - DC$  is the commutator, and  $\boldsymbol{\Omega}$  is the magnetic field.

Observe that,<sup>7</sup> by taking the trace, eq. (2)

$$\begin{aligned} \mathcal{D}_{\mathbf{p}} f_{\mathbf{p}}^c = & \sum_g \int w_{ep}(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p}) [f_{\mathbf{p}'}^c N_g - f_{\mathbf{p}}^c (N_g + 1)] \\ & + w_{ep}(\mathbf{p}'' \rightarrow \mathbf{p}, \mathbf{k}) (f_{\mathbf{p}''}^c (1 + N_g) - f_{\mathbf{p}}^c N_g) d\mathbf{k} + (\partial f_{\mathbf{p}}^c / \partial t)_{sf} \end{aligned} \quad (5)$$

(see Ref. 7).

### III. ASYMPTOTIC EXPANSION AND BALANCE EQUATIONS

Based on a suggestion of Akhiezer and Peletminski<sup>6</sup> (see also Ref. 7) we expand now the  $ep$ ,  $pe$ , and  $pp$  kernels and the unknowns with respect to a small parameter  $\epsilon$  which takes into account the effect of the umklapp (U) processes in addition to the normal (N) ones (which conserve momentum).

We start with electrons (the extension to phonons is trivial). The sought expansions for  $n_{\mathbf{p}}$  and  $N_g$  read

$$\mathbf{F}_{\mathbf{p}} = \mathbf{F}_{\mathbf{p}}^N + \epsilon \mathbf{F}_{\mathbf{p}}^U, \quad N_g = N_g^N + \epsilon N_g^U.$$

Accordingly

$$\left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{ep} = \left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{ep}^N + \epsilon \left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{ep}^U$$

and similarly for  $sf$  interactions. Now we introduce the following singular expansion for  $w_{tu}$  (dominant) and regular expansion for  $w_{sf}$ :

$$w_{tu} = (1/\epsilon) w_{rs}^N + w_{rs}^U,$$

$$w_{sf} = w_{sf}^N + \epsilon w_{sf}^U,$$

where  $tu = ep, pe, pp$ . We can write now

$$\left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{ep}^N = (1/\epsilon) \left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{ep}^{NN} + \left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{ep}^{NU},$$

$$\left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{ep}^U = (1/\epsilon) \left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{ep}^{UN} + \left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{ep}^{UU}.$$

$$\left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{sf}^N = \left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{sf}^{NN} + \epsilon \left( \frac{\partial \mathbf{F}_{\mathbf{p}}}{\partial t} \right)_{sf}^{NU},$$

$$\left(\frac{\partial \mathbf{F}_p}{\partial t}\right)_{sf}^U = \left(\frac{\partial \mathbf{F}_p}{\partial t}\right)_{sf}^{UN} + \epsilon \left(\frac{\partial \mathbf{F}_p}{\partial t}\right)_{sf}^{UU}.$$

By collecting all these terms, at the orders  $-1$  and  $0$ , we get

$$\begin{aligned} \left(\frac{\partial \mathbf{F}_p}{\partial t}\right)_{ep}^{NN} &= 0 \\ \left(\frac{\partial \mathbf{F}_p}{\partial t}\right)_{ep}^{NU} + \left(\frac{\partial \mathbf{F}_p}{\partial t}\right)_{ep}^{UN} & \\ + (i/2)[\boldsymbol{\Omega} \cdot \vec{\mathbf{S}}, \mathbf{F}_p^N] + \left(\frac{\partial \mathbf{F}_p}{\partial t}\right)_{sf}^{NN} &= \mathcal{D}_p \mathbf{F}_p^N \end{aligned} \quad (6)$$

respectively.

Analogously for phonons

$$\left(\frac{\partial N_g}{\partial t}\right)_{pp}^{NN} + \left(\frac{\partial N_g}{\partial t}\right)_{pe}^{NN} = 0$$

and

$$\begin{aligned} \left(\frac{\partial N_g}{\partial t}\right)_{pp}^{NU} + \left(\frac{\partial N_g}{\partial t}\right)_{pp}^{UN} + \\ \left(\frac{\partial N_g}{\partial t}\right)_{pe}^{NU} + \left(\frac{\partial N_g}{\partial t}\right)_{pe}^{UN} + \left(\frac{\partial N_g}{\partial t}\right)_{sf}^{NN} &= \mathcal{D}_g N_g^N. \end{aligned} \quad (7)$$

It can be verified that, by taking into account momentum and energy conservation, the equations of order  $-1$  for both phonons and electrons are solved by

$$N_g^N = \mathcal{B}[\beta(\omega_g - \mathbf{V} \cdot \mathbf{k})], \quad \mathbf{F}_p^N = \mathbf{A} \exp[\beta(-\mathcal{E}_p + \mathbf{V} \cdot \mathbf{p})],$$

where  $\beta = 1/T$  and

$$\mathcal{B}(\zeta) = 1/(e^\zeta - 1)$$

(Bose-Einstein distribution function), where the meaning of  $\mathbf{V}$  will become clear later on. Observe that, in order to solve *simultaneously*  $\mathbf{V}$  has to be the same for both electrons and phonons. However, a more refined model, with *two* values of  $\mathbf{V}$  have to be considered when the e-e interactions are accounted for.<sup>10</sup> As a consequence (see the appendix), we have also

$$\left(\frac{\partial f_p^c}{\partial t}\right)_{sf}^{NN} = 0, \quad \left(\frac{\partial N_g}{\partial t}\right)_{sf}^{NN} = 0.$$

By taking the trace of eq. (7) we have now

$$\left(\frac{\partial f_p^c}{\partial t}\right)_{ep}^{NU} + \left(\frac{\partial f_p^c}{\partial t}\right)_{ep}^{UN} = \mathcal{D}_p f_p^{cN}.$$

Equation (7) reduces to

$$\begin{aligned} \left(\frac{\partial N_g}{\partial t}\right)_{pp}^{NU} + \left(\frac{\partial N_g}{\partial t}\right)_{pp}^{UN} + \\ \left(\frac{\partial N_g}{\partial t}\right)_{pe}^{NU} + \left(\frac{\partial N_g}{\partial t}\right)_{pe}^{UN} &= \mathcal{D}_g N_g^N. \end{aligned}$$

We shall expand<sup>5</sup> now  $N_g^N$  and  $F_p^N$  as follows

$$N_g^N = \mathcal{B}(\beta\omega_g) - \beta\mathbf{V} \cdot \mathbf{k}\mathcal{B}'(\beta\omega_g) = N_g^e + N_g^o,$$

$$F_p = A \exp(-\mathcal{E}_p/T)(1 + \mathbf{V} \cdot \mathbf{p}/T) = F_p^e + F_p^o,$$

where we separated the symmetric component (e), which is even with respect to momentum and the anti-symmetric component (o), which is odd. This simplification will be justified *a posteriori* in the frame of the drift-diffusion approximation. Observe that

$$A = N/M_0(T),$$

where

$$N = \int F_p d\mathbf{p}, \quad M_0(T) = \int \exp(-\mathcal{E}_p/T) d\mathbf{p}.$$

Moreover we can write

$$f_p^{cN} = \text{tr}F_p^N = (n_c/M_0) \exp(-\mathcal{E}_p/T)(1 + \mathbf{V} \cdot \mathbf{p}) = f_p^{co} + f_p^{ce},$$

where  $n_c = \text{tr}N$  is the charge density, or, alternatively,

$$f_p^c = \exp(-(\mathcal{E}_p - \mu)/T)(1 + \mathbf{V} \cdot \mathbf{p})$$

where  $\mu = T \ln(n_c/M_0)$  is the chemical potential. Since

$$\int \mathbf{v} f_p^{co} d\mathbf{p} = -\beta(n_c/M_0) \int \mathbf{V} \cdot \mathbf{p} \exp(-\beta\mathcal{E}_p/T) \mathbf{v} d\mathbf{p}$$

$$= (n_c/M_0) \int \mathbf{V} \cdot \mathbf{p} \frac{\partial}{\partial \mathbf{p}} \exp(-\beta\mathcal{E}_p) d\mathbf{p} = \mathbf{V} \int f_p^{ce} d\mathbf{p},$$

the average velocity of electrons  $\langle \mathbf{v} \rangle$  [(see (4)], defined by

$$\langle \mathbf{v} \rangle = \int \mathbf{v} f_p^{cN} d\mathbf{p} / \int f_p^{cN} d\mathbf{p} = \int \mathbf{v} f_p^{co} d\mathbf{p} / \int f_p^{ce} d\mathbf{p},$$

is simply given by  $\mathbf{V}$ , and similarly for phonons. After some calculations we obtain

$$(\partial N_g / \partial t)_{pp}^{NU} = \beta\mathbf{V} \cdot \left\{ \int [(1/2) \sum_{g_1 g_2} (1 + N_g^e) N_{g_1}^e N_{g_2}^e w_{pp}^U(\mathbf{k}_1, \mathbf{k}_2 \rightarrow \mathbf{k})(\mathbf{k}_2 + \mathbf{k}_1 - \mathbf{k}) \right.$$

$$\left. + \sum_{g_1 g_3} (1 + N_{g_3}^0) N_g^e N_{g_1}^e w_{pp}^U(\mathbf{k}, \mathbf{k}_1 \rightarrow \mathbf{k}_3)(-\mathbf{k}_3 + \mathbf{k}_1 + \mathbf{k})] d\mathbf{k}_1 \right\},$$

$$(\partial N_g / \partial t)_{pe}^{NU} = \beta\mathbf{V} \cdot \left\{ \int f_p^{ce} (1 + N_{g_1}^e) w_{pe}^U(\mathbf{p} \rightarrow \mathbf{p}', \mathbf{k})(\mathbf{p} - \mathbf{k} - \mathbf{p}') d\mathbf{p} \right\}$$

and

$$(\partial f_p^c / \partial t)_{ep}^{NU} = \beta\mathbf{V} \cdot \left\{ \sum_g \int f_{p'}^{ce} N_g^e w_{ep}^U(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p})(\mathbf{k} + \mathbf{p}' - \mathbf{p}) \right.$$

$$\left. + f_{p'}^{ce} (1 + N_g^0) w_{ep}^U(\mathbf{p}' \rightarrow \mathbf{p}, \mathbf{k})(\mathbf{p}' - \mathbf{k} - \mathbf{p}) \right\} d\mathbf{k}.$$

Since  $w_{rs}^U = w_{rs} - w_{rs}^N$ , in the last three equations  $w_{rs}^U$  can be substituted by  $w_{rs}$ , due to momentum conservation for N-processes.

The equations of order 0 are the starting point of our macroscopic model. By projecting the electron one over 1 the continuity equation for electrons reads

$$\frac{\partial}{\partial t} \int F_p^e d\mathbf{p} + \nabla \cdot \int \mathbf{v} F_p^e d\mathbf{p} =$$

$$\int [(i/2)[\boldsymbol{\Omega} \cdot \vec{\mathcal{S}}, F_p^N] + \left( \frac{\partial F_p}{\partial t} \right)_{sf}^{NN}] d\mathbf{p} \quad (8)$$

By projecting the electron equation over  $\mathbf{p}$  and the phonon equations on  $\mathbf{k}$ , summation gives the following balance equation for momentum:

$$\begin{aligned} & \frac{\partial}{\partial t} \left( \int f_{\mathbf{p}}^{co} \mathbf{p} d\mathbf{p} + \int N_g^o \mathbf{k} d\mathbf{k} \right) \\ & + \nabla \cdot \left( \int f_{\mathbf{p}}^{ce} \mathbf{v} \otimes \mathbf{p} d\mathbf{p} + \sum_g \int N_g^e \mathbf{u}_g \otimes \mathbf{k} d\mathbf{k} \right) = \\ & -e\mathbf{E} \int f_{\mathbf{p}}^{ce} d\mathbf{p} + \int \left( \frac{\partial f_{\mathbf{p}}^c}{\partial t} \right)_{ep}^{NU} \mathbf{p} d\mathbf{p} + \\ & \int \left[ \sum_g \left( \frac{\partial N_g}{\partial t} \right)_{pp}^{NU} + \int \left( \frac{\partial N_g}{\partial t} \right)_{pe}^{NU} \right] \mathbf{k} d\mathbf{k}, \end{aligned} \quad (9)$$

where we took advantage of

$$\int \left( \frac{\partial f_{\mathbf{p}}^c}{\partial t} \right)_{ep}^{UN} \mathbf{p} d\mathbf{p} + \sum_g \int \left[ \left( \frac{\partial N_g}{\partial t} \right)_{pp}^{UN} + \int \left( \frac{\partial N_g}{\partial t} \right)_{pe}^{UN} \right] \mathbf{k} d\mathbf{k} = 0,$$

due to momentum conservation for N-processes.

Finally, by projecting the electron equation over  $\mathcal{E}_{\mathbf{p}}$  and the phonon ones over  $\omega_g$ , summation gives the following balance equation for energy

$$\begin{aligned} & \frac{\partial}{\partial t} \left( \int \mathcal{E}_{\mathbf{p}} f_{\mathbf{p}}^{ce} d\mathbf{p} + \sum_g \int \omega_g N_g^e d\mathbf{k} \right) + \\ & + \nabla \cdot \left( \int \mathbf{v} \mathcal{E}_{\mathbf{p}} f_{\mathbf{p}}^{co} d\mathbf{p} + \sum_g \int \mathbf{u}_g \omega_g N_g^o d\mathbf{k} \right) = -e\mathbf{E} \cdot \int \mathbf{v} f_{\mathbf{p}}^{co} d\mathbf{p}. \end{aligned} \quad (10)$$

More explicitly

$$\begin{aligned} & \frac{\partial}{\partial t} \left[ \frac{n_c \mathbf{V}}{M_0 T} \cdot \mathbb{M}_2(T) - \beta \mathbf{V} \cdot \sum_g \int \mathbf{k} \otimes \mathbf{k} \mathcal{B}'(\beta \omega_g) d\mathbf{k} \right] \\ & + \nabla(T n_c) + \nabla \cdot \sum_g \int \mathbf{u}_g \otimes \mathcal{B}(\beta \omega_g) \mathbf{k} d\mathbf{k} = -e\mathbf{E} n_c + \beta \mathbb{D} \cdot \mathbf{V}, \\ & \frac{\partial}{\partial t} \left[ -\frac{T^2 n_c}{M_0} + \sum_g \int \omega_g N_g d\mathbf{k} \right] + \\ & \nabla \cdot \left[ n_c T (1 - T M'_0 / M_0) \mathbf{V} - \beta \mathbf{V} \cdot \sum_g \int \mathbf{k} \otimes \mathbf{u}_g \omega_g \mathcal{B}'(\beta \omega_g) d\mathbf{k} \right] = -e n_c \mathbf{E} \cdot \mathbf{V}, \end{aligned}$$

where

$$\mathbb{M}_2(T) = \int \mathbf{p} \otimes \mathbf{p} \exp(-\beta \mathcal{E}_{\mathbf{p}}) d\mathbf{p}$$

and the tensor  $\mathbb{D}$ , can be written in the following symmetric form

$$\begin{aligned} \mathbb{D} = & -\frac{1}{2} \sum_{g_1 g_2 g_3} \int \int N_{g_2}^e N_{g_3}^e (1 + N_{g_1}^e) w_{pp}(\mathbf{k}_2, \mathbf{k}_3 \rightarrow \mathbf{k}_1) (\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \otimes (\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) d\mathbf{k}_1 d\mathbf{k}_2 \\ & - \sum_g \int \int f_{\mathbf{p}}^{ce} (1 + N_g^e) w_{ep}(\mathbf{p} \rightarrow \mathbf{p}', \mathbf{k}) (\mathbf{p} - \mathbf{k} - \mathbf{p}') \otimes (\mathbf{p} - \mathbf{k} - \mathbf{p}') d\mathbf{p} d\mathbf{k}. \end{aligned}$$

#### IV. THE EQUATIONS OF SPINTRONICS

By splitting  $N$  as

$$N = n_c I/2 + \mathbf{n}_s \cdot \vec{S}$$

(where  $n_c$  and  $\mathbf{n}_s$  are the charge and spin densities), eq. (8) gives:

$$\frac{\partial n_c}{\partial t} + \nabla \cdot (\mathbf{V} n_c) = 0$$

and, after some calculations (see also the appendix),

$$\begin{aligned} \frac{\partial \mathbf{n}_s}{\partial t} + \nabla \cdot (\mathbf{V} \otimes \mathbf{n}_s) = \\ -[1/M_0(T)] \left[ \mathbf{V} \cdot \int \mathbf{p} \otimes \boldsymbol{\Omega}_o \exp(-\mathcal{E}_p/T) \frac{d\mathbf{p}}{T} \right. \\ \left. + \int \boldsymbol{\Omega}_e \exp(-\mathcal{E}_p/T) d\mathbf{p} \right] \times \mathbf{n}_s - \mathbf{n}_s / \tau_{sf}(T) \end{aligned}$$

(here  $\boldsymbol{\Omega}_e$  and  $\boldsymbol{\Omega}_o$  are the even and odd components of  $\boldsymbol{\Omega}$ , respectively). This equation describes the precession of  $\mathbf{n}_s$  around the effective magnetic field (in square brackets) and its damping due to  $sf$  effects ( $\tau_{sf}(T)$  is the relaxation time).

Observe that this equation accounts now for a general dispersion relation.

#### V. CONCLUSIONS

New macroscopic equations are proposed for the semiconductor spintronics, which account for the new features summarized in the introduction. The equation for the spin density include the effects of the spin-orbit interaction (according to the known models) and of the spin-flip processes.

The new hydrodynamical model for electron-phonon systems we propose which is certainly related to the extended thermodynamical one.<sup>1,9(a),9(b)</sup> However the treatment resorts here strictly to kinetic theory, so that the model is closed. This means that we do not need adjustment of some free parameters (namely the relaxation times) by means of comparisons with Monte Carlo calculations.

Observe that the asymptotic expansion we introduce is valid ( $\epsilon \ll 1$ ) when the room temperature is much lower than the Debye temperature (in silicon, for example). An evolution equation for the spin density has been constructed, based on a new model which treats spin-flip processes as induced by interactions with phonons.

#### APPENDIX

Usually a spin-flip term is introduced in the spinor equation for electrons in a very simplified way which account that the spin distribution function vanishes at equilibrium. An appropriate time constant  $\tau_{sf}$  accounts for this process as follows

$$(\partial \mathbf{F}_p / \partial t)_{sf} = [(1/2)I(\text{tr} \mathbf{F}_p) - \mathbf{F}_p] / \tau_{sf},$$

which gives

$$(\partial n_c / \partial t)_{sf} = 0, \quad (\partial \mathbf{n}_s / \partial t)_{sf} = -\mathbf{n}_s / \tau_{sf}. \quad (\text{A1})$$

The present new model is derived from first principles. The spin-flip process is due to absorption/emission of phonons and appropriate collision integrals are constructed for both electrons and phonons. Let

$$\mathbf{F}_p^* = (1/2) f_p^c I - \mathbf{f}_p^s \cdot \vec{S}$$



be the spin-flipped distribution function. We propose the following model:

$$(\partial F_{\mathbf{p}}/\partial t)_{sf} = \sum_g \int \{w_{sf}(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p})F_{\mathbf{p}'}^* N_g - F_{\mathbf{p}}(N_g + 1) + w_{sf}(\mathbf{p}'' \rightarrow \mathbf{p}, \mathbf{k})[F_{\mathbf{p}''}^*(1 + N_g) - F_{\mathbf{p}} N_g]\} d\mathbf{k},$$

which gives

$$(\partial f_{\mathbf{p}}^c/\partial t)_{sf} = \sum_g \int \{w_{sf}(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p})[f_{\mathbf{p}'}^c N_g - f_{\mathbf{p}}^c(N_g + 1) + w_{sf}(\mathbf{p}'' \rightarrow \mathbf{p}, \mathbf{k})[f_{\mathbf{p}''}^c(1 + N_g) - f_{\mathbf{p}}^c N_g]\} d\mathbf{k},$$

and

$$(\partial \mathbf{f}_{\mathbf{p}}^s/\partial t)_{sf} = - \sum_g \int \{w_{sf}(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p})[\mathbf{f}_{\mathbf{p}'}^s N_g + \mathbf{f}_{\mathbf{p}}^s(N_g + 1) + w_{sf}(\mathbf{p}'' \rightarrow \mathbf{p}, \mathbf{k})[\mathbf{f}_{\mathbf{p}''}^s(1 + N_g) + \mathbf{f}_{\mathbf{p}}^s N_g]\} d\mathbf{k}.$$

Moreover for phonons we write

$$(\partial N_g/\partial t)_{sf} = \int w_{sf}(\mathbf{p} \rightarrow \mathbf{p}', \mathbf{k})(f_{\mathbf{p}}^c(1 + N_g) - f_{\mathbf{p}'}^c N_g) d\mathbf{p}.$$

Observe that

$$(\partial f_{\mathbf{p}}^c/\partial t)_{sf} \quad \text{and} \quad (\partial N_g/\partial t)_{sf}$$

have the same form as

$$(\partial f_{\mathbf{p}}^c/\partial t)_{ep} \quad \text{and} \quad (\partial N_g/\partial t)_{pe},$$

respectively, so that if the last two vanish, at the same time the first two vanish. Finally we can write

$$(\partial n_c/\partial t)_{sf}^{NN} = 0, \quad (\partial \mathbf{n}_s/\partial t)_{sf}^{NN} = -\mathbf{n}_s/\tau_{sf}, \quad (\text{A2})$$

where

$$1/\tau_{sf} = (2/M_0) \sum_g \int \int (N_g^e + 1)[w_{sf}(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p}) \exp(-\mathcal{E}_{\mathbf{p}}/T) + w_{sf}(\mathbf{p}'' \rightarrow \mathbf{p}, \mathbf{k}) \exp(-\mathcal{E}_{\mathbf{p}''}/T)] d\mathbf{k} d\mathbf{p}.$$

The present result (A2) agrees with the old one (A1), but here  $\tau_{sf}$  is now is given as a function of  $T$ .

- <sup>1</sup> A. M. Anile and S. Pennisi, "Thermodynamic derivation of the hydrodynamical model for charge transport in semiconductors," *Phys. Rev. B* **46**(20), 13186 (1992).
- <sup>2</sup> R. El Hajj, These, Doctorat de l'Universite' de Toulouse, "Etude mathematique et numerique de modeles de transport: application a la spintronique," 2008.
- <sup>3</sup> (a) A. Rossani, "Generalized kinetic theory of electrons and phonons," *Physica A* **305**, 323 (2002); (b) A. Rossani, G. Spiga, and A. Domaingo, "Band-trap capture and emission in the generalized kinetic theory of electrons and holes," *J. Phys. A* **36**, 11955 (2003); (c) A. Rossani and G. Spiga, "Auger effect in the generalized kinetic theory of electrons and holes," *J. Math. Phys.* **47**, 013301 (2006); (d) A. Rossani and A. M. Scarfone, "Generalized kinetic theory of electrons and phonons: models, equilibrium, stability," *Physica B* **334**, 292 (2003); (e) A. Rossani, "Generalized balance equations for an electron-phonon system," *J. Phys. A* **43**, 165002 (2010).
- <sup>4</sup> (a) N. Ben Abdallah, P. Degond, and S. Genyeis, "An energy-transport model for semiconductors derived from the Boltzmann equation," *J. Stat. Phys.* **84**(1-2), 205 (1996); (b) N. Ben Abdallah and P. Degond, "On a hierarchy of macroscopic models for semiconductors," *J. Math. Phys.* **37**(7), 3306 (1996);
- <sup>5</sup> M. Lundstrom, *Fundamentals of carrier transport* (CUP, Cambridge, 2000).
- <sup>6</sup> A. Akhiezer and S. Peletminski, *Les methodes de la Physique statistique* (Editions Mir, Moscou, 1980).
- <sup>7</sup> E. M. Lifshitz and L. P. Pitaevskii, *Physical Kinetics* (Pergamon Press, Oxford, 1981).
- <sup>8</sup> J. M. Ziman, *Electrons and phonons* (Clarendon Press, Oxford, 1960).
- <sup>9</sup> (a) V. Romano and M. Zwierz, "Electron-phonon hydrodynamical model for semiconductors," *Z. Angew. Math. Phys.* **61**, 1111-1131 (2010); (b) V. Romano and A. Rusakov, "2D numerical simulations of an electron-phonon hydrodynamical model based on the maximum entropy principle," *Computer methods in Applied Mechanics and Engineering* **199**, 2741-2751 (2010).
- <sup>10</sup> A. Rossani, "Modeling of the non-equilibrium effects by high electric fields in small semiconductor devices," *Physica A* **390**, 3329-3336 (2011).