Nonequilibrium Spin Magnetization Quantum Transport
Equations: Spin and Charge Coupling

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Abstract

The classical Bloch equations of spin magnetization transport is extended to fully time-dependent and highly-nonlinear nonequilibrium spin magnetization quantum distribution function transport (SMQDFT) equations. The relevant variables are the spinor correlation functions which separate into charge and spin magnetization distributions that becomes highly coupled in SMQDFT equations. The leading terms consist of the Boltzmann kinetic equation with spin-orbit coupling in a magnetic field together with spin-dependent scattering terms which contribute to the torque. These do not have analogue within the classical relaxation-dephasing picture, but are inherently quantum many-body effects. These should incorporate the spatio–temporal-dependent phase-space dynamics of Elliot-Yafet and D’yakonov-Perel scatterings. The resulting SMQDFT equations should serve as a theoretical foundation for computational spintronic and nanomagnetic device applications, in ultrafast-switching-speed/low-power performance and reliability analyses.
The ultrafast-switching-speed and power-dissipation performance analyses of nanoelectronic devices has revealed the inadequacy of the classical Boltzmann transport equation (BTE) and ushered its extension of the to fully time-dependent and highly-nonlinear nonequilibrium quantum distribution function (QDF) transport equations for charge carriers. This has been achieved through the use of non-equilibrium Green’s function, obtained either by the time-contour quantum field formulation of Schwinger[1], Keldysh[2], and Kadanoff and Baym[3], or by the real-time quantum superfield formulation of Buot coupled with his lattice Weyl (LW) transformation technique[4–7]. The extension of BTE to QDF transport equation has proved to be highly crucial in discovering autonomous current oscillations in resonant tunneling devices through numerical simulations, and in resolving controversial issues concerning highly-nonlinear and bistable current-voltage characteristics found in the experiments[9, 10]. Indeed, the QDF approach in phase space has so far been the most successful technique in the time-dependent analyses of open and active nanosystem and nanodevices[10].

To the authors’ knowledge, the extension of the well-known classical Bloch equation for spin transport, which is the analogue of the classical BTE for particle transport, to fully time-dependent and highly-nonlinear nonequilibrium QDF transport equations for the magnetization has not been reported. With the exploding surge of interest on spintronics and nanomagnetics[11], there is an urgent need for this fully quantum transport extension of the classical Bloch equation to guide the numerical simulation of the speed-power switching performance of realistic spin nanostructures/transistors. The well-known classical Bloch equations for spin systems is usually given in the diffusive regime[12] as

\[
\begin{align*}
\frac{\partial M_x}{\partial t} & = \left[ D \nabla^2 M_x - \frac{M_x}{T_2} \right] + \gamma \left( \vec{M} \times \vec{B} \right)_x, \\
\frac{\partial M_y}{\partial t} & = \left[ D \nabla^2 M_y - \frac{M_y}{T_2} \right] + \gamma \left( \vec{M} \times \vec{B} \right)_y, \\
\frac{\partial M_z}{\partial t} & = \left[ D \nabla^2 M_z - \frac{M_z - M_o}{T_1} \right] + \gamma \left( \vec{M} \times \vec{B} \right)_z, 
\end{align*}
\]

(1)

where \( \gamma \) is the gyromagnetic ratio, \( T_1 \) is the spin-relaxation characteristic time, and \( T_2 \) is the spin-dephasing characteristic time.

The purpose of this paper is to extend this classical Bloch equations to a fully time-dependent and highly-nonlinear nonequilibrium SMQDFT equations on the same level as in the extension of the classical BTE to full QDF transport equation based on nonequilibrium
Green’s function technique\cite{1–6}. In this paper we will first treat spin transport within a single energy band. The multiband spin transport, where pseudo-spin plays a role, will be reported in a separate arxiv.org online paper.

Our starting point is the general quantum transport expressions for fermions, as obtained from the real-time quantum superfield theoretical technique\cite{5, 6}. Upon dropping the Cooper pairing terms in those expressions which do not concern us in this paper (their corresponding transport equations\cite{5, 6} are important in nonequilibrium superconductivity), the nonequilibrium Green’s function transport equations reduce to the following known expressions\cite{1–3},

\[
i\hbar \left( \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} \right) G^\zeta = [v G^\zeta - G^\zeta v^T] + [\Sigma^r G^\zeta - G^\zeta \Sigma^a] + [\Sigma^\zeta G^a - G^\zeta \Sigma^\zeta] .
\]

(2)

The quantum distribution-function transport equations in \((p, q) = (p, q, E, t)\)-space are obtained by applying the LW transformation\cite{7} (although continuum approximation is employed in this paper, this is not essential and we use the word ”lattice” when referring to solid-state problems)\cite{5, 6}. The LW transform \(a(p, q)\) of any operator \(\hat{A}\) is defined by the following relation

\[
a(p, q) = \int dv \exp \left( \frac{ip \cdot v}{\hbar} \right) \langle q - \frac{v}{2} | \hat{A} | q + \frac{v}{2} \rangle \equiv \mathcal{W} (v, \tau, q, t) ,
\]

(3)

where the matrix element in the integrand is evaluated between two Wannier functions, and \(\mathcal{W}\) indicates the operation of taking the LW transform. This transformation enables the numerical simulation of real time-dependent dynamical open systems by transforming from two-point correlation functions to numerically manageable and physically meaningful local functions in phase space\cite{8}. The well-known electron Wigner distribution function (WDF), \(f_w (p, q, t)\), is obtained from the correlation function \(-i\hbar G^<\) by performing integration over the energy variable

\[
f_w (p, q, t) = \frac{1}{2\pi \hbar} \int dE \ (-i\hbar G^< (p, E, q, t)) .
\]

(4)

In the absence of particle pairing of superconductivity to obtain Eq. \(2\), we may also write the general transport equation, written for \('<'\)-quantities as [here \(\{A, B\}\) and \(\{B, A\}\]
means anticommutator and commutator, respectively, of $A$ and $B$],

$$
i\hbar \left( \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} \right) G^<
= \left[ \tilde{H}, G^< \right] + [\Sigma^<, \text{Re } G^r] - \frac{i}{2} \{\Gamma, G^<\} + \frac{i}{2} \{\Sigma^<, A\}, \tag{5}
$$

where the single-particle Hamiltonian,

$$\tilde{H} = H_o + \Sigma^\delta + \text{Re } \Sigma^r,$$

with $\Sigma^\delta$ being the 'singular part' (delta function in time) of the self-energy.

$$H_o = E(p) + V(q),$$

where $E(p)$ is the electron dispersion relation or energy-band function and $V(q)$ is the self-consistent single-particle potential function. In obtaining Eq. (5) from Eq. (2), we made use of the relations, $(G^a)\dagger = G^r$, and $\Sigma^\ell(1, 2) = -\Sigma^<(2, 1)$, and the following relations, $iA(1, 2) = -2i \text{Im } G^r = - (G^>(1, 2) - G^<(1, 2))$, $i\Gamma(1, 2) = -2i \text{Im } \Sigma^r = - (\Sigma^>(1, 2) - \Sigma^<(1, 2)).$

The second term in Eq. (5) is a commutator and also describes evolution in phase-space although only serving to complicate, by virtue of the scattering term, $\Sigma^<$, the kinetics of particle motion described by the first term, a sort of complex interference phenomena similar to *zitterbewegung* in Dirac quantum mechanics[13]. Although often neglected in considering quantum transport of particles as this is expected to make a small corrections to the particle current, we will include the $[\Sigma^<, \text{Re } G^r]$ term in our present considerations for completeness. Note that in the gradient expansion of Eq. (5), with the $[\Sigma^<, \text{Re } G^r]$ term neglected, the leading terms immediately give the classical Boltzmann transport equation for spinless systems[14]. However, even this is no longer quite true for spin system as we shall see later, since the spinor scattering terms contribute to the torque in the system.

The third term of Eq. (5), which is proportional to $G^<$, is the *scattering-out* term, and the last term which is proportional to the spectral density is the *scattering-in* term, in analogy with the collision terms in the classical Boltzmann equation. The collision terms can also be rewritten using the identity,

$$-\frac{i}{2} \{\Gamma, G^<\} + \frac{i}{2} \{\Sigma^<, A\} = -\frac{1}{2} \{\Sigma^<, G^>\} + \frac{1}{2} \{\Sigma^>, G^<\}.$$
which also leads to \( i \Sigma^> \) and \( -i \Sigma^< \) terms, upon performing the \( \mathcal{W} \) operation, as scattering-out and scattering-in collision terms, respectively \[3\].

The equation for \( G^r \) and \( G^a = G^{r\dagger} \) are simpler and are given as, 
\[
\dot{G}^{-1}G^{r} = 0, \quad G^{a} \left( \dot{G}^{-1} \right)^{\dagger} = 0,
\]
where
\[
\dot{G}^{-1}G^{r} (1, 2) = i\hbar \left( \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} \right) G^{r} (1, 2) - \left[ \mathcal{H} + \Sigma^r, G^{r} \right] (1, 2).
\]

The above equations are then cast in the language of phase-space QDF transport equations, similar to that of the classical Boltzmann equation by the use of Buot lattice Weyl-Wigner formulation of the band dynamics of electrons in a solid \[7\]. In the \textit{continuum approximation}, the first thing to do is to recast the \textit{two-point} space and time arguments in all the transport equations as follows: \( t_1 = t - \frac{\tau}{2}, \ t_2 = t + \frac{\tau}{2}, \ q_1 = q - \frac{v}{2}, \ q_2 = q + \frac{v}{2}. \) We also need to define a \((3 + 1)\)-dimensional canonical variables, namely, \( p = (p, -E), \ q = (q, t), \) which allows us to write \( v = (v, \tau). \) The transformation of Eq. \[3\] is then applied.

For simplicity in spin quantum transport equations, we consider only a single energy band having spin indices, \( \downarrow \) and \( \uparrow. \) Incorporating the \( \downarrow \) and \( \uparrow \) variables in Eqs. \[2\] and \[5\], we obtain exactly four transport equations for \( G^<_{\uparrow\uparrow} (1, 2), \ G^<_{\uparrow\downarrow} (1, 2), \ G^<_{\downarrow\uparrow} (1, 2), \) and \( G^<_{\downarrow\downarrow} (1, 2). \) In spintronics, we are interested in the time-dependent evolution of the magnetic polarization, \( S_z = i\hbar \left( G^<_{\uparrow\uparrow} - G^<_{\downarrow\downarrow} \right), \) as this is transported across the device. In order to achieve this, we need to perform \textit{linearly-independent} combinations of the components of the spinor nonequilibrium Green’s function consisting of the set: \( \{G^<_{\uparrow\uparrow} (1, 2), G^<_{\uparrow\downarrow} (1, 2), G^<_{\downarrow\uparrow} (1, 2), G^<_{\downarrow\downarrow} (1, 2)\}. \) The resulting new set will become the relevant and independent correlation functions more pertinent to the spin-transport problem, which consists of the separation into charge distribution and spin magnetization vector.

The separation in terms of a scalar and vector representing the total charge and spin-vector correlation functions, naturally occurs as expansion coefficient in terms of the Pauli matrices,
\[
\begin{pmatrix}
  G^<_{\uparrow\uparrow} & G^<_{\uparrow\downarrow} \\
  G^<_{\downarrow\uparrow} & G^<_{\downarrow\downarrow}
\end{pmatrix}
= \frac{1}{2} \left( S_o \mathcal{I} + \vec{S} \cdot \vec{\sigma} \right),
\]
where $\hat{I}$ is the $2 \times 2$ identity matrix, and

$$
S_x = \left( G_{\uparrow\uparrow}^{<} + G_{\downarrow\downarrow}^{<} \right),
$$

$$
iS_y = \left( G_{\uparrow\downarrow}^{<} - G_{\downarrow\uparrow}^{<} \right),
$$

$$
S_z = \left( G_{\uparrow\uparrow}^{<} - G_{\downarrow\downarrow}^{<} \right),
$$

$$
S_\sigma = \left( G_{\uparrow\uparrow}^{<} + G_{\downarrow\downarrow}^{<} \right),
$$

(7)

where we drop the '$<$' superscript in the spin correlation functions, $S_j$. In the frame of reference where the $z$ direction is fixed by the magnetic field, the $S_x$ and $S_y$ evolution equation describe *dephasing* mechanisms in the $x$-$y$ plane of the 'Bloch sphere'. The total charge of the system, $\rho(p, q, t)$ is represented by the scalar $S_\sigma$, i.e., from Eq. (4) we have,

$$
\rho(\vec{q}, t) = \frac{1}{2(2\pi\hbar)^2} \int d\vec{p} \, dE \left( -i\hbar S_\sigma(\vec{p}, E, \vec{q}, t) \right),
$$

(8)

where $S_\sigma(\vec{p}, E, \vec{q}, t)$ is the LW of correlation $S_\sigma$. Thus Eq. (6) performs the separation of the charge and spin correlation functions as the relevant variables of any fermion system with spin degree of freedom.

For slowly varying systems where the total charge vary slowly with space and time, perhaps in some spin transfer torque systems, we can reduce the number of important spin correlation functions in the spin quantum transport problem by making an approximation to $S_\sigma$. Assuming the conservation of particles possessing spin degree of freedom within semiconductor channel of, say, a spintronic transfer torque transistor, we must have the following relation for the $\uparrow\uparrow$ and $\downarrow\downarrow$ rates of change,

$$
\frac{\partial \rho_{\uparrow\uparrow}(p, q, t)}{\partial t} = -\frac{\partial \rho_{\downarrow\downarrow}(p, q, t)}{\partial t},
$$

where $\rho_{\uparrow\uparrow}(p, q, t)$ and $\rho_{\downarrow\downarrow}(p, q, t)$ are the LW transforms of $\hbar G_{\uparrow\uparrow}^{<}$ and $\hbar G_{\downarrow\downarrow}^{<}$, respectively.

Generally however, $S_\sigma$ will be varying in both space and time, i.e., a two-point nonequilibrium correlation function in space and time, describing the varying charge within the spintronic device due to depletion and accumulation in various regions within the device, such as in spin transfer torque devices employing thin barriers between the channel and ferromagnetic leads.

We can also write the spinor self-energies used in Eq. (2) as into spin-independent scalar [denoted by overscript bar symbol] and vector quantities,

$$
\Sigma_{\alpha\beta}^{a,r,\sigma} = \frac{1}{2} \left( \Sigma_{\alpha\beta}^{a,r,\sigma} \hat{I} + \Xi_{\alpha\beta}^{a,r,\sigma} \cdot \vec{\sigma} \right),
$$

6
which we write explicitly as,

\[ \Sigma_{\alpha\beta} = \frac{1}{2} \left( \begin{array}{cc}
\bar{\Sigma}^r + \Xi_z^r & \Xi_x^r - i\Xi_y^r \\
\Xi_x^r + i\Xi_y^r & \bar{\Sigma}^r - \Xi_z^r
\end{array} \right), \]

\[ \Sigma^a_{\alpha\beta} = \frac{1}{2} \left( \begin{array}{cc}
\bar{\Sigma}^a + \Xi_z^a & \Xi_x^a - i\Xi_y^a \\
\Xi_x^a + i\Xi_y^a & \bar{\Sigma}^a - \Xi_z^a
\end{array} \right), \]

\[ \Sigma^{\langle}_{\alpha\beta} = \frac{1}{2} \left( \begin{array}{cc}
\bar{\Sigma}^{\langle} + \Xi_z^{\langle} & \Xi_x^{\langle} - i\Xi_y^{\langle} \\
\Xi_x^{\langle} + i\Xi_y^{\langle} & \bar{\Sigma}^{\langle} - \Xi_z^{\langle}
\end{array} \right). \]

Likewise, the spinor quantities used in Eq. (5), namely, the spin-dependent scattering-out \( \Gamma \) term is cast in the form,

\[ \frac{\Gamma_{\alpha\beta}}{2} = \frac{1}{2} \left( \bar{\Gamma} \hat{I} + \vec{\gamma} \cdot \vec{\sigma} \right) = -\text{Im} \Sigma_{\alpha\beta}^r = -\frac{1}{2} \left( \text{Im} \Sigma^r \hat{I} + \text{Im} \bar{\Xi} \cdot \vec{\sigma} \right), \]  

(9)

so that

\[ \bar{\Gamma} = -\text{Im} \Sigma^r, \]

\[ \vec{\gamma} = -\text{Im} \bar{\Xi}. \]  

(10)

Similarly, we have for the spin-dependent spectral function, \( A \), in the scattering-in term as

\[ \frac{A_{\alpha\beta}}{2} = \frac{1}{2} \left( \bar{A} \hat{I} + \vec{A} \cdot \vec{\sigma} \right) = -\text{Im} S_{\alpha\beta}^r = -\frac{1}{2} \left( \text{Im} \bar{S} \hat{I} + \text{Im} \bar{\Xi} \cdot \vec{\sigma} \right), \]  

(11)

so that

\[ \bar{A} = -\text{Im} \bar{S}^r, \]

\[ \vec{A} = -\text{Im} \bar{\Xi}. \]  

(12)

In the effective-mass approximation, we may take the corresponding single-particle Hamiltonian \( \hat{H}_s \) for spin systems in a magnetic field with spin-orbit coupling as

\[ \hat{H}_s = \left( \frac{\hat{P}^2}{2m^*} - eV \langle q \rangle + \frac{1}{2} \text{Re} \Sigma^r \right) \hat{I} + H_{so} \left( \hat{P}, \hat{Q} \right) + \frac{1}{2} \left( \text{Re} \bar{\Sigma} \cdot \vec{\sigma} - g_{eff} \mu_B \vec{B} \cdot \vec{\sigma} \right), \]  

(13)
where \( \hat{P} = \hat{P} + \frac{e}{\hbar} A(q) \), electric charge, \( e = |e| \), \( V(q) \) is the self-consistent applied potential, and \( \vec{B} = \nabla_q \times A(q) \). The second term, \( H_{so}(\hat{P}, \hat{Q}) \), is the spin-orbit coupling which may consists of Dresselhaus and/or Rashba term[18] as well as transistor-gate and strain-induced spin-orbit coupling. The term \( \Re \vec{\Sigma}r \cdot \vec{\sigma} \) comes from the spin vector of the spin-dependent part of \( \Re \Sigma_{a\beta} \) in the single particle Hamiltonian. Its presence basically modifies the effective magnetic field due to external fields and spin-orbit coupling.

We have in general,

\[
H_{so}(\hat{P}, \hat{Q}) = \mu_B \frac{\vec{q} \times \hat{P}}{2\hbar m^* c^2} \left| \frac{\vec{E}}{q} \right| \cdot \vec{\sigma},
\]

which may acquire definite form in lower dimensional system based on symmetry considerations[18]. In what follows, we write the most general form of the single-particle Hamiltonian, \( \hat{H}_s \), as

\[
\hat{H}_s = \frac{1}{2} \left( H \left( \hat{P}, \hat{Q} \right) \hat{I} - \vec{h} \cdot \vec{\sigma} \right),
\]

where \( \vec{h} \left( \hat{P}, \hat{Q} \right) = \left( g_s \frac{e}{2mc} \vec{B}_{eff} - \Re \vec{\Sigma}r \right) \). Therefore

\[
\hat{H}_s = \frac{1}{2} \left( \hat{H} \hat{I} - \vec{\sigma} \cdot \vec{B} \right),
\]

where

\[
\vec{B} = g_s \frac{e}{2mc} \vec{B}_{eff},
\]

and for electron-spin angular momentum, the \( g \)-factor, \( g_s \simeq 2 \). Here the effective \( \vec{B}_{eff} \left( \hat{P}, \hat{Q} \right) \) includes the effects of transistor-gate or strain induced spin-orbit coupling, and applied magnetic fields. \( H \left( \hat{P}, \hat{Q} \right) \) consists of the energy-band structure and spin-independent confining potential due to the device heterostructure coupled with the applied bias at the terminals. The spin-orbit coupling in \( \vec{B}_{eff} \left( \hat{P}, \hat{Q} \right) \) also depends very much on the electric field of the self-consistent potential inside the device. This in turn depends on the total electric charge, represented by \( S_o \), through the Poisson equation. Although we could include \( \Re \vec{\Sigma}r \) in the definition of \( \vec{B} \) above, we treat this separately to emphasize the possible role of scattering terms in contributing to the torque in the system.

The resulting equations obeyed by the spin correlation functions defined by Eq. (7) in

\[
\text{(14)}
\]
accordance with Eq. (2) can be written in vector notation as,

\[
\frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} \bar{S}^\prec
\]

\[
= \frac{1}{2} \left[ \bar{H}, \bar{S}^\prec \right] + \frac{1}{2} \left[ \Sigma^r \bar{S}^\prec - \bar{S}^\prec \Sigma^a \right] + \frac{1}{2} \left[ \bar{\Sigma} \bar{S}^a - \bar{S}^a \bar{\Sigma} \right]
\]

\[
+ \frac{i}{2} \left[ \bar{B} \times \bar{S}^\prec - \bar{S}^\prec \times \bar{B} \right]
\]

\[
+ \frac{1}{2} \left[ \bar{\xi}^r \times \bar{S}^\prec - \bar{S}^\prec \times \bar{\xi}^a \right] + \frac{i}{2} \left[ \bar{\xi}^a \times \bar{S}^a - \bar{S}^a \times \bar{\xi} \right]
\]

\[
+ \frac{1}{2} \left[ \bar{\Xi} \bar{S}^a < S_o < - S_o < \bar{\Xi}^a ] + \frac{i}{2} \left[ \bar{\Xi}^a \times \bar{S}^a - \bar{S}^a \times \bar{\Xi}^a \right]
\]

\[
+ \frac{1}{2} \left[ \bar{\Xi}^a \times \bar{S}^a - \bar{S}^a \times \bar{\Xi}^a \right],
\]

(16)

and for the scalar correlation function representing the total charge,

\[
\frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} S_o^<
\]

\[
= \frac{1}{2} \left[ \bar{H}, S_o^< \right] + \frac{1}{2} \left[ \Sigma^r S_o^< - S_o^< \Sigma^a \right] + \frac{1}{2} \left[ \bar{\Sigma} S_o^a - S_o^a \bar{\Sigma} \right]
\]

\[
+ \frac{1}{2} \left[ \bar{\Xi} \cdot \bar{S}^< - \bar{S}^< \cdot \bar{\Xi} \right] + \frac{1}{2} \left[ \bar{\Xi}^r \cdot \bar{S}^< - \bar{S}^< \cdot \bar{\Xi}^a \right]
\]

\[
+ \frac{1}{2} \left[ \bar{\Xi}^a \cdot \bar{S}^a - \bar{S}^a \cdot \bar{\Xi}^a \right].
\]

(17)

For self-consistency, one must also be solved for potential, \( \Phi \), or electric field, \( \bar{E} \), using the Poisson equation,

\[
\nabla^2 \Phi = e \frac{\rho(q,t) - \rho_o}{\varepsilon_o},
\]

where \( \Phi = V \) in Eq. (13), \( \rho_o \) is the positive background charge and \( \rho(q,t) \) is given by Eq. (8).

We also have the equivalent equation for \( \bar{S}^\prec \),

\[
\frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} \bar{S}^\prec
\]

\[
= \frac{1}{2} \left[ \bar{H} + \text{Re} \Sigma^r, \bar{S}^\prec \right] + \frac{i}{2} \left\{ \text{Im} \Sigma^r, \bar{S}^\prec \right\} - \frac{i}{2} \left\{ \Sigma^r, \text{Im} \bar{S}^r \right\} + \left[ \Sigma^r, \text{Re} \bar{S}^r \right]
\]

\[
+ \frac{i}{2} \left[ \left( \bar{\Xi} \right)^r \times \bar{S}^\prec - \bar{S}^\prec \times \left( \bar{\Xi} \right)^r \right]
\]

\[
- \frac{i}{2} \left\{ \text{Im} \bar{\Xi}^r \times \bar{S}^\prec + \bar{S}^\prec \times \text{Im} \bar{\Xi}^r \right\} + \frac{i}{2} \left\{ \bar{\Xi}^r \times \text{Im} \bar{S}^r + \text{Im} \bar{S}^r \times \bar{\Xi}^r \right\}
\]

\[
+ \frac{i}{2} \left\{ \bar{\Xi}^a \times \text{Re} \bar{S}^r - \text{Re} \bar{S}^r \times \bar{\Xi}^a \right\}
\]

\[
+ \frac{1}{2} \left[ \bar{\Xi}, S_o^< \right] + \frac{i}{2} \left\{ \text{Im} \bar{\Xi}^r, S_o^< \right\} + \frac{i}{2} \left\{ \bar{\Xi}^r, \text{Re} S_o^r \right\} - \frac{i}{2} \left\{ \bar{\Xi}^a, \text{Im} S_o^a \right\},
\]

(18)

which can be reduced to that which one can derive from Eq. (5), by using the relations in Eqs. (10) and (12). The result is
\[ i\hbar \left( \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} \right) \vec{S}^< \]
\[ = \frac{1}{2} \left[ \vec{H} + \text{Re } \Sigma^r, \vec{S}^< \right] - \frac{i}{2} \left\{ \vec{\gamma}, \vec{S}^< \right\} + \frac{i}{2} \left\{ \Sigma^<, \vec{A} \right\} + \left[ \Sigma^<, \text{Re } \vec{S}^r \right] \]
\[ + \frac{i}{2} \left[ \left( \vec{B} + \text{Re } \vec{\Xi}^r \right) \times \vec{S}^< - \vec{S}^< \times \left( \vec{B} + \text{Re } \vec{\Xi}^r \right) \right] \]
\[ + \frac{1}{2} \left\{ \vec{\gamma} \times \vec{S}^< + \vec{S}^< \times \vec{\gamma} \right\} - \frac{1}{2} \left\{ \vec{\Xi}^< \times \vec{A} + \vec{A} \times \vec{\Xi}^< \right\} \]
\[ + \frac{i}{2} \left[ \vec{\Xi}^< \times \text{Re } \vec{S}^r - \text{Re } \vec{S}^r \times \vec{\Xi}^< \right] \]
\[ + \frac{1}{2} \left[ \left( \vec{B} + \text{Re } \vec{\Xi}^r \right), S^<_o \right] + \left[ \vec{\Xi}^<, \text{Re } S^<_o \right] - \frac{i}{2} \left\{ \vec{\gamma}, S^<_o \right\} - \frac{i}{2} \left\{ \vec{\Xi}^<, \text{Im } S^<_o \right\} \]. \tag{19} \]

Note that our definition of \( \vec{B} \), Eq. (15), has the unit of energy, just like the self-energies.

The equivalent expression derived from Eq. (5) in terms of the magnetization vector, \( \vec{M} = g_s \mu_B \vec{S} \) (the g-factor for spin, \( g_s \approx 2 \)) is,
\[ i\hbar \left( \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} \right) \vec{M} \]
\[ = \frac{1}{2} \left[ \vec{H} + \text{Re } \Sigma^r, \vec{M} \right] - \frac{i}{2} \left\{ \vec{\gamma}, \vec{M} \right\} + \frac{i}{2} g_s \mu_B \left\{ \Sigma^<, \vec{A} \right\} + \frac{1}{2} \left[ \Sigma^<, \text{Re } \vec{M}^r \right] \]
\[ + \frac{i}{2} \left[ \left( \vec{B} + \text{Re } \vec{\Xi}^r \right) \times \vec{M} - \vec{M} \times \left( \vec{B} + \text{Re } \vec{\Xi}^r \right) \right] \]
\[ + \frac{1}{2} \left\{ \vec{\gamma} \times \vec{M} + \vec{M} \times \vec{\gamma} \right\} - \frac{1}{2} g_s \mu_B \left\{ \vec{\Xi}^< \times \vec{A} + \vec{A} \times \vec{\Xi}^< \right\} \]
\[ + \frac{i}{2} \left[ \vec{\Xi}^< \times \text{Re } \vec{M}^r - \text{Re } \vec{M}^r \times \vec{\Xi}^< \right] \]
\[ + \frac{1}{2} \left[ \left( \vec{B} + \text{Re } \vec{\Xi}^r \right), M^<_o \right] + \frac{1}{2} \left[ \vec{\Xi}^<, \text{Re } M^<_o \right] - \frac{i}{2} \left\{ \vec{\gamma}, M^<_o \right\} - \frac{i}{2} \left\{ \vec{\Xi}^<, \text{Im } M^<_o \right\} \]. \tag{20} \]

where we defined,
\[ \vec{M}^r = g_s \mu_B \vec{S}^r, \]
\[ M^<_o = g_s \mu_B S^<_o. \]

First, let us evaluate Eqs. (20) by assuming constant magnetic field \( \vec{B} \) and in the absence of scatterings. We obtain
\[ \frac{\partial}{\partial t} \vec{M} \]
\[ = \mathcal{W} \left\{ \frac{1}{i\hbar} \left[ \vec{H}, \vec{M} \right] + \frac{1}{\hbar} \vec{M} \times \vec{B} \right\}, \tag{21} \]

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which is the ballistic version of the form of Eq. (1).

In carrying out the LW transform, the following relations between vector cross products and commutation or anti-commutation relations are useful,

\[
\vec{A} \times \vec{B} - \vec{B} \times \vec{A} = \hat{I}_i \hat{\epsilon}_{ijk} \{A_j, B_k\},
\]

\[
\vec{A} \times \vec{B} + \vec{B} \times \vec{A} = \hat{I}_i \hat{\epsilon}_{ijk} [A_j, B_k],
\]

where \(\hat{I}_i\) is the unit dyadic symmetric tensor or \textit{idemfactor}, and \(\hat{\epsilon}_{ijk}\) is the anti-symmetric unit tensor. For the purpose of making gradient expansion to make contact with classical expressions, we give here the following for convenience the LW transform of a commutator \([A, B]\) and an anticommutator \(\{A, B\}\) in terms of Poisson bracket differential operator, \(\Lambda\), as

\[
[A, B] (p, q) = \cos \Lambda \left[ a (p, q) b (p, q) - b (p, q) a (p, q) \right] - i \sin \Lambda \left\{ a (p, q) b (p, q) + b (p, q) a (p, q) \right\}, \tag{22}
\]

\[
\{A, B\} (p, q) = \cos \Lambda \left\{ a (p, q) b (p, q) + b (p, q) a (p, q) \right\} - i \sin \Lambda \left[ a (p, q) b (p, q) - b (p, q) a (p, q) \right], \tag{23}
\]

where \(\Lambda = \frac{\hbar}{2} \left( \frac{\partial^{(a)}}{\partial p} \cdot \frac{\partial^{(b)}}{\partial q} - \frac{\partial^{(a)}}{\partial q} \cdot \frac{\partial^{(b)}}{\partial p} \right)\). Thus if the LW transforms are not matrices, then to lowest order, we have

\[
[A, B] (p, q) = -i \frac{\hbar}{2} \left( \frac{\partial a (p, q)}{\partial p} \cdot \frac{\partial b (p, q)}{\partial q} - \frac{\partial a (p, q)}{\partial q} \cdot \frac{\partial b (p, q)}{\partial p} \right), \tag{24}
\]

\[
\{A, B\} (p, q) = \left\{ a (p, q) b (p, q) + b (p, q) a (p, q) \right\} = 2 a (p, q) b (p, q). \tag{25}
\]

If we compare Eqs. (16)-(19) with the particle quantum transport equation of Eq. (5), without the \textit{zitterbewegung} \([\Sigma^<, \text{Re} G^n]\) term, we see that the leading terms of the first line of the RHS of Eq. (19), corresponds to the classical BTE. The next three lines give the torque, due to spin-orbit coupling (included in the effective magnetic field), and terms coming from the spin-dependent relaxation and dephasing scattering mechanisms. The last line explicitly involves coupling to the total charge.

Carrying out the \(W\) operation in Eq. (20), we find that the leading gradient terms in the
RHS reads

\[
\left( \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} \right) \vec{M} = -\frac{1}{m} \left( \vec{p} + \frac{e}{c} \vec{A}(q) \right) \cdot \nabla_q \vec{M} - e \left( \vec{E} + \frac{1}{2c} (\vec{v} \times \vec{B}) \right) \cdot \nabla_{p'} \vec{M} - \frac{e}{mc} \Sigma < \vec{A} + \frac{1}{h} \vec{B} \times \vec{M} \\
- \frac{1}{2} \left[ \frac{\partial \text{Re} \Sigma^r}{\partial p} \frac{\partial \vec{M}}{\partial q} - \frac{\partial \text{Re} \Sigma^r}{\partial q} \frac{\partial \vec{M}}{\partial p} \right] - \frac{1}{2} \left[ \frac{\partial \Sigma^<}{\partial p} \frac{\partial \text{Re} \vec{M}^r}{\partial q} - \frac{\partial \Sigma^<}{\partial q} \frac{\partial \text{Re} \vec{M}^r}{\partial p} \right] \\
+ \frac{1}{h} \text{Re} \vec{\Xi}^r \times \vec{M} + \frac{1}{h} \vec{\Xi}^< \times \text{Re} \vec{M}^r \\
- \frac{1}{2} \tilde{I} \varepsilon_{ijk} \left[ \frac{\partial \gamma_j}{\partial p} \frac{\partial M_{k}^o}{\partial q} - \frac{\partial \gamma_j}{\partial q} \frac{\partial M_{k}^o}{\partial p} \right] + \frac{1}{2 mc} \tilde{I} \varepsilon_{ijk} \left[ \frac{\partial \Xi_j}{\partial p} \frac{\partial A_{k}}{\partial q} - \frac{\partial \Xi_j}{\partial q} \frac{\partial A_{k}}{\partial p} \right] \\
- \frac{1}{2} \left[ \frac{\partial \vec{B}}{\partial q} \frac{\partial M_{o}^<}{\partial p} - \frac{\partial \vec{B}}{\partial p} \frac{\partial M_{o}^<}{\partial q} \right] - \frac{1}{h} \vec{\gamma} M_{o}^< - \frac{1}{h} \vec{\Xi}^< \text{Im} M_{o}^r \\
- \frac{1}{2} \left[ \frac{\partial \text{Re} \vec{\Xi}^r}{\partial p} \frac{\partial M_{o}^<}{\partial q} - \frac{\partial \text{Re} \vec{\Xi}^r}{\partial q} \frac{\partial M_{o}^<}{\partial p} \right] - \frac{1}{2} \left[ \frac{\partial \Xi^<}{\partial p} \frac{\partial \text{Re} M_{o}^r}{\partial q} - \frac{\partial \Xi^<}{\partial q} \frac{\partial \text{Re} M_{o}^r}{\partial p} \right],
\]

(26)

where all quantities above are LW transforms, i.e., they are functions defined in phase space \((p, q, t) = (\vec{p}, -E, \vec{q}, t)\). In the first line of Eq. (26) and the first term of the second line arise from the relation,

\[
- \frac{1}{2} \left[ \frac{\partial (\vec{H} + \text{Re} \Sigma^r)}{\partial p} \frac{\partial \vec{M}}{\partial q} - \frac{\partial (\vec{H} + \text{Re} \Sigma^r)}{\partial q} \frac{\partial \vec{M}}{\partial p} \right] \\
= -\frac{1}{m} \left( \vec{p} + \frac{e}{c} \vec{A}(q) \right) \cdot \nabla_q \vec{M} - e \left( \vec{E} + \frac{1}{2c} (\vec{v} \times \vec{B}) \right) \cdot \nabla_{p'} \vec{M} \\
- \frac{1}{2} \left[ \frac{\partial \text{Re} \Sigma^r}{\partial p} \frac{\partial \vec{M}}{\partial q} - \frac{\partial \text{Re} \Sigma^r}{\partial q} \frac{\partial \vec{M}}{\partial p} \right],
\]

(27)

where the RHS arise from the expression given by the first terms of Eq. (13). We have used the gauge: \(\vec{A}(q) = \left( \frac{1}{2} \vec{B} \times \vec{q} \right)\), \(\vec{B}\) is the uniform external magnetic field. We have used the gauge: \(\vec{A}(q) = \left( \frac{1}{2} \vec{B} \times \vec{q} \right)\), \(\vec{B}\) is the uniform external magnetic field. We have used the gauge: \(\vec{A}(q) = \left( \frac{1}{2} \vec{B} \times \vec{q} \right)\), \(\vec{B}\) is the uniform external magnetic field.

The first line in the RHS of Eq. (26) is the Boltzmann equation in a magnetic field with effects of spin-orbit coupling. The second line is the contribution to the Boltzmann equation if the effects of \(\text{Re} \Sigma^r\) and \(\text{Re} \vec{M}^r\) are included. The rest of this equation incorporates spin-dependent scattering, \(\text{Re} \vec{\Xi}^r\), which directly contribute to the torque. The precession of the magnetic moment, \(\vec{M}\), is also correlated with the torque exerted by \(\vec{\gamma}\), and similarly for 'scattering-in' precession (fluctuation) of \(\vec{A}\) due to torque exerted by \(\vec{\Xi}\). The last two lines describe the coupling to the total charge. Thus, spin-dependent scattering terms are capable of describing the spatio–temporal-dependent scattering dynamics of various mechanisms of spin relaxations and precession, namely, Elliott-Yafet (spin-dependent impurities
and phonon scatterings), D'yakonov-Perel’ (due to electron-electron scatterings, with electrons executing random-walk in momentum space, resulting in the fluctuations of magnitude and direction of spin precession axis). The Bir-Aronov-Pikus scattering (due to the interaction with holes in valence band, serving as a spin sink), and the hyperfine interactions are not relevant in our present treatment.

Until now the treatments of spin transport are mainly focused on scattering mechanisms, based on quasi-classical steady-state conditions and/or where nonuniformity in real space is often not considered, common in micromagnetics. On the other hand for spintronic transistor devices, strong inhomogeneity in real space is of prime considerations. The calculations of the self energy $\Sigma$ often have the goal of obtaining the relaxation times to be used in classical kinetic equations.

A calculation where the self-energy spinor due to many-body effects of spin-orbit coupling is treated has been given by Rajagopal\cite{21}. A first principle \textit{ab initio} calculation of the self-energies has been given by Zhukov and Chulkov\cite{22} for the Elliot-Yafet mechanism in Al, Cu, Au, Nb, and Ta, and by Mower, Vignale, and Tokatly\cite{23} for D’yakonov-Perel spin relaxation mechanism in photo-excited electron-hole liquid in intrinsic semiconductors exhibiting spin-split band structure.

Our derivation of the nonequilibrium spin magnetization QDF transport equations is based on the separation of charge and spin as the relevant variables. The resulting SMQDFT equations should provide the fundamental basis for carrying out the numerical simulation of the switching or time-dependent performance analyses of spintronic devices, such as those that make use of thin insulating layers between conducting metal layers\cite{24}. Potential barriers of up to 1 eV exist in promising spintronic devices, exemplified by the spin valve and magnetic tunnel transistors\cite{25, 26}.

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[8] In contrast to Fourier transformation, the matrix element in the integrand of Eq. (3) which is diagonal in either lattice position or crystal momentum is invariant under the lattice Weyl transformation. Clearly, the crystal momentum and lattice position themselves, considered as matrix element of momentum and position operator, respectively, are invariant under lattice Weyl transformation.

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It is worth mentioning that the transformation from four independent operators or quantum states to their four linearly-independent combinations has yielded some of the deepest concepts of quantum mechanics, namely, spin angular momentum and quantum teleportation. A two-state eigenvector space, denoted by basis $|\uparrow\rangle$ and $|\downarrow\rangle$, has the following complete set of four basis operators, $\hat{b}_{\downarrow\uparrow} = |\downarrow\rangle \langle \uparrow|$, $\hat{b}_{\uparrow\downarrow} = |\uparrow\rangle \langle \downarrow|$, $\hat{d}_{\downarrow\downarrow} = |\downarrow\rangle \langle \downarrow|$, and $\hat{d}_{\uparrow\uparrow} = |\uparrow\rangle \langle \uparrow|$. The spin operators are obtained as simple linear combinations of the above basis operators as, $\hat{S}_o = \frac{\hbar}{2} (\hat{d}_{\downarrow\downarrow} + \hat{d}_{\uparrow\uparrow})$, $\hat{S}_x = \frac{\hbar}{2} (\hat{b}_{\downarrow\uparrow} + \hat{b}_{\uparrow\downarrow})$, $\hat{S}_y = \frac{\hbar}{2} (\hat{b}_{\downarrow\uparrow} - \hat{b}_{\uparrow\downarrow})$, $\hat{S}_z = \frac{\hbar}{2} (\hat{d}_{\downarrow\downarrow} - \hat{d}_{\uparrow\uparrow})$, obeying the quantum-mechanical spin angular-momentum commutation relations, namely, $[\hat{S}_j, \hat{S}_k] = i\hbar \epsilon_{jkl} \hat{S}_l$, $i, j, k \neq o$. In matrix form, these are represented by the well-known Pauli matrix, $\vec{\sigma}$, namely, $\hat{S}_x = \frac{\hbar}{2} \sigma_x$, $\hat{S}_y = \frac{\hbar}{2} \sigma_y$, $\hat{S}_z = \frac{\hbar}{2} \sigma_z$. Note that operator $\hat{S}_o$ represent the identity operator (by virtue of the completeness relation for the eigenvectors; statistically referred to as a pure state) multiplied by $\frac{\hbar}{2}$. Any $2 \times 2$ matrix in 'spin' space can be expanded in terms of the Pauli and identity operators.

We note further that the linear combination of product states in a two-qubit system generates the entanglement Bell basis states which play a crucial role in the theory of quantum teleportation.[6, 20].

For example, for symmetric quantum well, the Rashba spin-orbit coupling can be expressed as $H_R = \frac{\alpha}{\hbar} (\hat{e}_z \times \vec{p}) \cdot \vec{\sigma}$, where $\alpha$ is the Rashba spin-orbit parameter.

In taking the derivative of $\frac{\partial H}{\partial q}$, we make the expansion of kinetic energy terms in $\vec{H} \Rightarrow \frac{\vec{p}^2}{2m} + \frac{e}{mc} \vec{p} \cdot \vec{A} + \left(\frac{e}{mc}\right)^2 \vec{A} \cdot \vec{A}$ using the symmetric Landau gauge: $\vec{A} = \frac{1}{2} (\vec{B} \times \vec{q})$. Then in taking the gradient with respect to $\vec{q}$, the $\vec{A} \cdot \vec{A}$ term does not contribute and we are left with,

$$\frac{e}{mc} \vec{p} \cdot \frac{\partial}{\partial q} \vec{A} = \frac{e}{mc} \vec{p} \cdot \frac{\partial}{\partial q} \left(\frac{1}{2} (\vec{B} \times \vec{q})\right)$$

$$= -\frac{e}{mc} \frac{1}{2} \vec{p} \cdot \frac{\partial}{\partial q} (\vec{q} \times \vec{B}) = -\frac{e}{mc} \frac{1}{2} \vec{p} \cdot \left(\hat{I} \times \vec{B}\right)$$

$$= -\frac{e}{mc} \frac{1}{2} (\vec{p} \times \vec{B}) = -\frac{e}{2c} (\vec{v} \times \vec{B})$$

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