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Spin polarization effects and their time evolutions

A. Vernes[a] and P. Weinberger[b*]

[a]*Austrian Center of Competence for Tribology, Viktor-Kaplan-Strasse 2, 2700 Wiener Neustadt, Austria;* [b]*Center for Computational Nanoscience, Seilerstätte 10/21, 1010 Vienna, Austria*

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The time evolution of the density corresponding to the polarization operator, originally constructed to commute with the Dirac Hamiltonian in the absence of an external electromagnetic field, is investigated in terms of the time-dependent Dirac equation taking the presence of an external electromagnetic field into account. It is found that this time evolution leads to 'tensorial' and 'vectorial' particle current densities and to the interaction of the spin density with the external electromagnetic field. As the time evolution of the spin density does not refer to a constant of motion (continuity condition) it only serves as auxiliary density. By taking the non-relativistic limit, it is shown that the polarization, spin and magnetization densities are independent of electric field effects and, in addition, no preferred directions can be defined.

1. Introduction

In quite a few experimental set-ups, nowadays, fast pulses of probing fields are applied to record the change in the physical properties of systems of interest. Very often it is found that these changes occur on the time scale of a few nano- or picoseconds, or even femtoseconds when using ultrafast laser pulses.[1] Usually, the recorded quantity refers to a change in electric or magneto-optical properties by measuring time-dependent resistances (resistivities) or, e.g. time-dependent Kerr signals.[2] Usually, because of the lack of theoretical concepts, in the case of changes in the magnetic properties, the experimental results are then interpreted using phenomenological models such as, for example, variations of the Landau–Lifshitz–Gilbert (LLG) equation in terms of parameters partially or totally deduced from experiments.

In this paper, we derive in detail a quantum mechanically correct description [3] of the time evolution of the polarization density by considering the time-dependent Dirac equation in the presence of an external electromagnetic field. In particular, in Section 2, we first introduce the well-known spin operator, the Dirac operator with and without electromagnetic field and discuss the necessity for using the so-called polarization operator in Section 3, since (even) the relativistic spin density is not a well-defined quantity. The derivation of the time evolution of the polarization density, formulated in Section 4, will lead to a set of coupled equations that as an auxiliary quantity contains the spin density, whose time evolution therefore needs also to be considered (Section 5). The significance and formal

*Corresponding author. Email: peter@pwein.at

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structure of the occurring *vectorial* and *tensorial* particle current densities are then explained in Section 6. Considering in Section 7, the time evolution of the magnetization density, it will turn out that this density is independent of electric field effects.

Finally, in Section 8, the usefulness of a bispinor representation immediately becomes obvious when considering the non-relativistic limit: not only is the time evolution of the non-relativistic polarization density independent of the electric field, the corresponding non-relativistic spin and magnetization densities, related to each other only by the Bohr magneton, cannot be associated with any particular (polarization) direction, since the Pauli spin matrices are SU2 invariant [4]. Exactly because of these obvious deficiencies of the non-relativistic polarization and spin densities, the present approach is important for interpretations of experiments using fast electromagnetic field pulses.

Last, but not least in Section 9, a scheme to evaluate approximately the time evolution of various densities in terms of time-dependent density functional theory (TDFT) and instantaneous time-dependent resolvents [5] is recalled.

It is essential to point out right from the beginning that – as will be shown – within a non-relativistic description, no experiment in which an electric field is applied can be explained nor can there be any directional preference be specified for the time evolution of the spin density.

2. Dirac Hamiltonians and the spin operator

As is probably well known, the spin operator $\vec{\boldsymbol{\Sigma}}$,

$$\vec{\boldsymbol{\Sigma}} = \begin{pmatrix} \vec{\boldsymbol{\sigma}} & 0 \\ 0 & \vec{\boldsymbol{\sigma}} \end{pmatrix},$$

is not a constant of motion of the Dirac Hamilton operator $\mathcal{H}_0$,

$$\begin{aligned} \mathcal{H}_0 = c\vec{\boldsymbol{\alpha}} \cdot \vec{\boldsymbol{p}} + \boldsymbol{\beta} m_{\mathrm{e}} c^2 \,, \; \left[\mathcal{H}_0, \vec{\boldsymbol{\Sigma}}\right]_- \neq 0, \\ \vec{\boldsymbol{\alpha}} = \begin{pmatrix} 0 & \vec{\boldsymbol{\sigma}} \\ \vec{\boldsymbol{\sigma}} & 0 \end{pmatrix}, \; \boldsymbol{\beta} = \begin{pmatrix} \mathbf{I}_2 & 0 \\ 0 & -\mathbf{I}_2 \end{pmatrix}, \end{aligned} \tag{1}$$

where the commutator $[a, b]_-$ denotes the expression $ab - ba$. Therefore, also Σ_μ,

$$\Sigma_\mu \equiv (\vec{\boldsymbol{\Sigma}}, \; \Sigma_4) = (\vec{\boldsymbol{\Sigma}}, -i\, \boldsymbol{\gamma}_5), \; \boldsymbol{\gamma}_5 = \begin{pmatrix} 0 & -\mathbf{I}_2 \\ -\mathbf{I}_2 & 0 \end{pmatrix},$$

does not commute with the Dirac Hamilton operator $\mathcal{H}$ in the presence of an external electromagnetic field

$$\mathcal{H} \equiv \mathcal{H}(\vec{r}, t) = c\vec{\boldsymbol{\alpha}} \cdot \vec{\boldsymbol{\pi}} + \boldsymbol{\beta} m_{\mathrm{e}} c^2 + eV\mathbf{I}_4, \; \left[\mathcal{H}, \Sigma_\mu\right]_- \neq 0, \tag{2}$$

$$\vec{\boldsymbol{\pi}} = (\vec{\boldsymbol{p}} - e\vec{A})\mathbf{I}_4 \,, \; \vec{A} = \vec{A}(\vec{r}, t), \; V = V(\vec{r}, t). \tag{3}$$

Here, $\vec{\boldsymbol{\sigma}} = (\sigma_x, \sigma_y, \sigma_z)$ refers to the vector of Pauli matrices, $\mathbf{I}_n$ is an n-dimensional unit matrix, while $\vec{A}$ and V denote the vector and scalar potential, respectively. In the following, both, $\vec{A}$ and V, will be assumed to be Hermitian.

3. The polarization operator

The so-called (dimensionless) polarization operator [6,7] T_μ is defined by

$$T_\mu \equiv (\vec{T}, T_4) = \left(\boldsymbol{\beta}\, \vec{\boldsymbol{\Sigma}} + \boldsymbol{\gamma}_5 \frac{\vec{\boldsymbol{\pi}}}{m_e c}, i\, \vec{\boldsymbol{\Sigma}} \cdot \frac{\vec{\boldsymbol{\pi}}}{m_e c} \right), \tag{4}$$

and has the following properties [8],

$$\sum_{j=1}^{4} T_j T_j = 3\mathbf{I}_4 + \frac{e\hbar}{(m_e c)^2}\, \vec{\boldsymbol{\Sigma}} \cdot \vec{B} = 3\mathbf{I}_4 - \frac{2\mu_B}{m_e c^2}\, \vec{\boldsymbol{\Sigma}} \cdot \vec{B},$$

$$\begin{cases} \left[\vec{T}, \mathcal{H}\right]_- = 2i\mu_B \left[\vec{\boldsymbol{\Sigma}} \times \vec{B} - \dfrac{1}{c}\boldsymbol{\gamma}_5 \left(\vec{E} + \dfrac{\partial \vec{A}}{\partial t} \right) \right] \\ [T_4, \mathcal{H}]_- = -\dfrac{2\mu_B}{c}\, \vec{\boldsymbol{\Sigma}} \cdot \left(\vec{E} + \dfrac{\partial \vec{A}}{\partial t} \right) \end{cases}, \tag{5}$$

where $\vec{B}$ is the magnetic field (magnetic induction) and $\vec{E}$ is the electric field. From Equation (5), it easily can be read off that by construction in the absence of an external electromagnetic field T_μ commutes with $\mathcal{H}_0$,

$$\left[T_\mu, \mathcal{H}_0\right]_- = 0, \tag{6}$$

i.e. is a constant of motion. It should be noted that both T_μ and Σ_μ are covariant axial four vectors.

4. Time evolution of the polarization density

In the following, the polarization density $\mathcal{T}_\mu \equiv \mathcal{T}_\mu(\vec{r}, t)$

$$\mathcal{T}_\mu = (\vec{\mathcal{T}}, \mathcal{T}_4), \; \vec{\mathcal{T}} = \psi^+ \vec{T} \psi, \; \mathcal{T}_4 = \psi^+ T_4 \psi, \tag{7}$$

and the spin density $\mathcal{S}_\mu \equiv \mathcal{S}_\mu(\vec{r}, t)$

$$\mathcal{S}_\mu \equiv (\vec{\mathcal{S}}, \mathcal{S}_4), \; \vec{\mathcal{S}} = \psi^+ \vec{\boldsymbol{\Sigma}}\, \psi, \; \mathcal{S}_4 = \psi^+ \Sigma_4 \psi = i\psi^+ \gamma_5 \psi \tag{8}$$

refer to the solutions $\psi \equiv \psi(\vec{r}, t)$ and $\psi^+ \equiv \psi^+(\vec{r}, t)$ of the time-dependent Dirac equation,

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar}\mathcal{H}\psi, \; \frac{\partial \psi^+}{\partial t} = -\frac{1}{i\hbar}\psi^+ \mathcal{H}, \tag{9}$$

with $\mathcal{H}$ being defined in Equation (2). Because of the chain rule, the time evolution of the polarization density consists of three parts, namely

$$\frac{d\mathcal{T}_\mu}{dt} = \frac{\partial \psi^+}{\partial t} T_\mu \psi + \psi^+ \frac{\partial T_\mu}{\partial t} \psi + \psi^+ T_\mu \frac{\partial \psi}{\partial t},$$

which can immediately be rewritten in terms of Equation (9) as:

$$\frac{d\mathcal{T}_\mu}{dt} = \frac{1}{i\hbar} \psi^+ (T_\mu \mathcal{H} - \mathcal{H}^+ T_\mu) \psi + \psi^+ \frac{\partial T_\mu}{\partial t} \psi, \tag{10}$$

where now

$$\frac{\partial T_\mu}{\partial t} = \left(\frac{\partial \vec{T}}{\partial t}, \frac{\partial T_4}{\partial t} \right),$$

and according to Equation (4)

$$\frac{\partial \vec{T}}{\partial t} = \boldsymbol{\gamma}_5 \frac{e}{m_{\mathrm{e}}c}\frac{\partial \vec{A}}{\partial t}\ ,\quad \frac{\partial T_4}{\partial t} = -\frac{ie}{m_{\mathrm{e}}c}\ \vec{\boldsymbol{\Sigma}}\cdot\frac{\partial \vec{A}}{\partial t}. \tag{11}$$

Using the explicit form of $\mathcal{H}$ given in Equation (2) and T_μ as $(\vec{T}, T_4)$, from Equation (4), the various parts in Equation (10) can compactly be written as:

$$\begin{cases} i\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\left(\psi^+\vec{T}\psi\right) = c\psi^+\left[\vec{T}\left(\vec{\boldsymbol{\alpha}}\cdot\vec{\boldsymbol{\pi}}\right) - \left(\vec{\boldsymbol{\pi}}^+\cdot\vec{\boldsymbol{\alpha}}\right)\vec{T}\right]\psi \\ \qquad\qquad - 2c\psi^+\left(\boldsymbol{\gamma}_5\beta\vec{\boldsymbol{\pi}}\right)\psi - \dfrac{ie\hbar}{m_{\mathrm{e}}c}\vec{E}\psi^+\boldsymbol{\gamma}_5\psi \\ i\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\left(\psi^+T_4\psi\right) = c\psi^+\left[T_4\left(\vec{\boldsymbol{\alpha}}\cdot\vec{\boldsymbol{\pi}}\right) - \left(\vec{\boldsymbol{\pi}}^+\cdot\vec{\boldsymbol{\alpha}}\right)T_4\right]\psi \\ \qquad\qquad -\dfrac{e\hbar}{m_{\mathrm{e}}c}\psi^+\left(\vec{\boldsymbol{\Sigma}}\cdot\vec{E}\right)\psi \end{cases}, \tag{12}$$

where $\vec{\boldsymbol{\pi}}^+ = \left(-\vec{p} - e\vec{A}\right)\mathbf{I}_4$, see also Table 1. It is perhaps useful to recall that, e.g. the second and third term on the lhs of the first equation in Equation (12) arise in turn from the terms $\boldsymbol{\beta} m_{\mathrm{e}}c^2$ and $eV\mathbf{I}_4$ in Equation (2). Note also that the expression containing the electric field $\vec{E}$ is only of the order of c^{-1}.

Taking into account the explicit form of $\vec{T}$ and T_4, the below commutator relations follow from Equation (5) and Tables 1 and 2,

$$\begin{cases} \left[\vec{T}, \left(\vec{\boldsymbol{\alpha}}\cdot\vec{\boldsymbol{\pi}}\right)\right]_- = 2\boldsymbol{\gamma}_5\boldsymbol{\beta}\vec{\boldsymbol{\pi}} + \dfrac{ie\hbar}{m_{\mathrm{e}}c}\,\vec{\boldsymbol{\Sigma}}\times\vec{B} \\ \left[T_4, \left(\vec{\boldsymbol{\alpha}}\cdot\vec{\boldsymbol{\pi}}\right)\right]_- = 0 \end{cases},$$

Table 1. Commutators.

$\left[\beta\vec{\Sigma},\ \beta\right]_-$	$= \left[\beta\vec{\Sigma},\ V\right]_- = 0$
$\left[\beta\vec{\Sigma},\ \vec{\alpha}\cdot\vec{\pi}\right]_-$	$= [\gamma_5\vec{\pi},\ \beta]_- = 2\gamma_5\beta\vec{\pi}$
$[\gamma_5\vec{\pi},\ V]_-$	$= i\hbar\gamma_5\left(\vec{E} + \dfrac{\partial\vec{A}}{\partial t}\right)$
$[\gamma_5\vec{\pi},\ \vec{\alpha}\cdot\vec{\pi}]_-$	$= -ie\hbar\vec{\Sigma}\times\vec{B}$
$\left[\vec{\Sigma}\cdot\vec{\pi},\ V\right]_-$	$= i\hbar\vec{\Sigma}\cdot\left(\vec{E} + \dfrac{\partial\vec{A}}{\partial t}\right)$
$\left[\alpha_\mu,\ T_\nu\right]_-$	$= 2\delta_{\mu\nu}\beta\gamma_5\ ,\ (\mu,\ \nu = x,\ y,\ z)$
$[\vec{\alpha},\ T_4]_-$	$= 2\left(\dfrac{\vec{\pi}}{m_e c}\times\vec{\Sigma}\right)\gamma_5$

Table 2. Useful relations.

$\vec{\alpha}\otimes\vec{T}+\vec{T}\otimes\vec{\alpha}$	$=\vec{\Sigma}\otimes\dfrac{\vec{\pi}}{m_e c}+\dfrac{\vec{\pi}}{m_e c}\otimes\vec{\Sigma}$
$\vec{\alpha}\otimes\vec{T}-\vec{T}\otimes\vec{\alpha}$	$=2\beta\left(\vec{\Sigma}\otimes\vec{\Sigma}\right)\gamma_5+\vec{\Sigma}\otimes\dfrac{\vec{\pi}}{m_e c}-\dfrac{\vec{\pi}}{m_e c}\otimes\vec{\Sigma}$
$\vec{\alpha}T_4+T_4\vec{\alpha}$	$=-2i\dfrac{\vec{\pi}}{m_e c}\gamma_5$

Table 3. Approximate time evolution of various densities.

Operator O	Time evolution of	$\omega(r;t)$
1_4	Particle density	n
$\beta\vec{\Sigma}$	Magnetization density	$\vec{M}_e$
$\begin{cases}\vec{\Sigma}\\ \Sigma_4=\gamma_5\end{cases}$	Spin density	$\begin{cases}\vec{S}\\ -iS_4\end{cases}$
$\begin{cases}\vec{T}=\left(\beta\,\vec{\Sigma}+\gamma_5\dfrac{\vec{\pi}}{m_e c}\right)\\ T_4=i\,\vec{\Sigma}\cdot\dfrac{\vec{\pi}}{m_e c}\end{cases}$	Polarization density	$\begin{cases}\vec{T}\\ T_4\end{cases}$

and Equation (12) can immediately be reformulated as:

$$\begin{cases} i\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\left(\psi^+\vec{T}\psi\right)=\dfrac{ie\hbar}{m_\mathrm{e}}\psi^+\left(\vec{\boldsymbol{\Sigma}}\times\vec{B}\right)\psi-\dfrac{ie\hbar}{m_\mathrm{e}c}\vec{E}\,\psi^+\boldsymbol{\gamma}_5\psi \\ \qquad\qquad\qquad +c\psi^+\left[\left(\vec{\boldsymbol{\alpha}}\cdot\vec{\boldsymbol{\pi}}-\vec{\boldsymbol{\pi}}^+\cdot\vec{\boldsymbol{\alpha}}\right)\vec{T}\right]\psi \\ \\ i\hbar\dfrac{\mathrm{d}}{\mathrm{d}t}\left(\psi^+T_4\psi\right)=-\dfrac{e\hbar}{m_\mathrm{e}c}\psi^+\left(\vec{\boldsymbol{\Sigma}}\cdot\vec{E}\right)\psi \\ \qquad\qquad\qquad +c\psi^+\left[\left(\vec{\boldsymbol{\alpha}}\cdot\vec{\boldsymbol{\pi}}-\vec{\boldsymbol{\pi}}^+\cdot\vec{\boldsymbol{\alpha}}\right)T_4\right]\psi \end{cases}. \tag{13}$$

It is important to recall that the scalar product symbol refers to a traditionally used short-hand notation.

Consider, for example, only the term $\left(\vec{\boldsymbol{\pi}}^+\cdot\vec{\boldsymbol{\alpha}}\right)\vec{T}$ in Equation (13). Keeping in mind that $\left(\vec{\boldsymbol{\pi}}^+\cdot\vec{\boldsymbol{\alpha}}\right)=\left(\pi_x^+\alpha_x+\pi_y^+\alpha_y+\pi_z^+\alpha_z\right)$ and $\vec{T}=\left(T_x,T_y,T_z\right)$, then

$$\left(\vec{\boldsymbol{\pi}}^+\cdot\vec{\boldsymbol{\alpha}}\right)\vec{T}\equiv\vec{\boldsymbol{\pi}}^+\cdot\left(\vec{\boldsymbol{\alpha}}\otimes\vec{T}\right),$$

$$\vec{\boldsymbol{\alpha}}\otimes\vec{T}=\begin{pmatrix}\alpha_\mathrm{x}\\ \alpha_\mathrm{y}\\ \alpha_\mathrm{z}\end{pmatrix}\otimes\begin{pmatrix}T_\mathrm{x} & T_\mathrm{y} & T_\mathrm{z}\end{pmatrix},$$

where $\otimes$ denotes a *Kronecker* product of two vectors, whose elements are matrices: $\vec{\boldsymbol{\alpha}} \otimes \vec{T}$ is a 3×3 super matrix

$$\vec{\boldsymbol{\alpha}} \otimes \vec{\boldsymbol{T}} = \begin{pmatrix} \alpha_x T_x & \alpha_y T_x & \alpha_z T_x \\ \alpha_x T_y & \alpha_y T_y & \alpha_z T_y \\ \alpha_x T_z & \alpha_y T_z & \alpha_z T_z \end{pmatrix}, \tag{14}$$

of matrix elements

$$\alpha_\mu T_\nu = \begin{pmatrix} 0 & \sigma_\mu \\ \sigma_\mu & 0 \end{pmatrix} \begin{pmatrix} \sigma_\nu & 0 \\ 0 & \sigma_\nu \end{pmatrix}, \; \nu, \mu = \mathrm{x, y, z},$$

i.e. explicitly corresponds to a 12×12 square matrix.

As in Equation (13), the contribution from the vector potential $\vec{A}$ drops out, by recalling that $\vec{p} = -i\hbar\nabla$, one formally can write:

$$\begin{cases} \psi^+ \left[\left(\vec{\boldsymbol{\alpha}} \cdot \vec{\boldsymbol{\pi}} - \vec{\boldsymbol{\pi}}^+ \cdot \vec{\boldsymbol{\alpha}} \right) \vec{T} \right] \psi = -i\hbar\nabla \cdot \left[\psi^+ \left(\vec{\boldsymbol{\alpha}} \otimes \vec{T} \right) \psi \right] \\ \psi^+ \left[\left(\vec{\boldsymbol{\alpha}} \cdot \vec{\boldsymbol{\pi}} - \vec{\boldsymbol{\pi}}^+ \cdot \vec{\boldsymbol{\alpha}} \right) T_4 \right] \psi = -i\hbar\nabla \cdot \left[\psi^+ \left(\vec{\boldsymbol{\alpha}} T_4 \right) \psi \right] \end{cases}$$

and therefore, the time evolution of the polarization density can be cast in the form of

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} \left(\psi^+ \vec{T} \psi \right) + c\nabla \cdot \left[\psi^+ \left(\vec{\boldsymbol{\alpha}} \otimes \vec{T} \right) \psi \right] \\ \qquad = \dfrac{e}{m_e} \left(\psi^+ \vec{\boldsymbol{\Sigma}} \psi \right) \times \vec{B} - \dfrac{e}{m_e c} \vec{E}\, \psi^+ \boldsymbol{\gamma}_5 \psi \\ \dfrac{\mathrm{d}}{\mathrm{d}t} \left(\psi^+ T_4 \psi \right) + c\nabla \cdot \left[\psi^+ \left(\vec{\boldsymbol{\alpha}} T_4 \right) \psi \right] = \dfrac{ie}{m_e c} \left(\psi^+ \vec{\boldsymbol{\Sigma}} \psi \right) \cdot \vec{E} \end{cases} . \tag{15}$$

In the absence of an external electromagnetic field, both left sides equate to zero. In this particular case, Equation (15) reduces according to the Noether theorem to the continuity condition for the polarization density.

It should be noted that in using the relations for a permutation of the order of elements in the Kronecker product $\vec{\boldsymbol{\alpha}} \otimes \vec{T}$, see Table 1, one obtains a completely equivalent formulation for the time evolution of the polarization density, which finally can be written in a compact manner as:

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} \vec{\mathcal{T}} + \nabla \cdot \overleftrightarrow{\mathcal{J}} = \dfrac{e}{m_e} \vec{\mathcal{S}} \times \vec{B} - \dfrac{e}{m_e c} \vec{E}\, \mathcal{S}_4 \\ \dfrac{\mathrm{d}}{\mathrm{d}t} \mathcal{T}_4 + \nabla \cdot \vec{\mathcal{J}}_4 = \dfrac{ie}{m_e c} \vec{\mathcal{S}} \cdot \vec{E} \end{cases}, \tag{16}$$

where

$$\begin{cases} \overleftrightarrow{\mathcal{J}} = \overleftrightarrow{\mathcal{J}}^{(1)} + \overleftrightarrow{\mathcal{J}}^{(2)} \\ \vec{\mathcal{J}}_4 = \vec{\mathcal{J}}_4^{(1)} - \vec{\mathcal{J}}_4^{(2)} \end{cases}, \tag{17}$$

with

$$\begin{aligned} &\overleftrightarrow{\mathcal{J}}^{(1)} = c\,\psi^+ \left(\vec{T} \otimes \vec{\boldsymbol{\alpha}} \right) \psi, \; \overleftrightarrow{\mathcal{J}}^{(2)} = c\,\psi^+ \left(2\,\boldsymbol{\beta}\boldsymbol{\gamma}_5 \right) \psi, \\ &\vec{\mathcal{J}}_4^{(1)} = c\,\psi^+ \left(T_4 \vec{\boldsymbol{\alpha}} \right) \psi, \; \vec{\mathcal{J}}_4^{(2)} = c\,\psi^+ \left(\frac{\vec{\boldsymbol{\pi}}}{m_e c} \times \vec{\boldsymbol{\alpha}} \right) \psi, \end{aligned} \tag{18}$$

and $\vec{\mathcal{S}}$ and $\mathcal{S}_4$ were introduced in Equation (8), see also [3].

5. Time evolution of the spin density

Since on the rhs of Equation (16) the components of the spin density $\mathcal{S}_\mu$ occur, the time evolution of the polarization density cannot be obtained unless simultaneously the time evolution of $\mathcal{S}_\mu$ is evaluated. As a derivation of $d\mathcal{S}_\mu/\mathrm{d}t$ is similar to that for $d\mathcal{T}_\mu/\mathrm{d}t$, it is sufficient to quote here only the final result, namely

$$\left\{\begin{array}{l} \dfrac{\mathrm{d}}{\mathrm{d}t}\left(\psi^+\vec{\boldsymbol{\Sigma}}\psi\right) + c\nabla\cdot\left[\psi^+\left(\vec{\boldsymbol{\alpha}}\otimes\vec{\boldsymbol{\Sigma}}\right)\psi\right] = \dfrac{2c}{\hbar}\psi^+\left(\vec{\boldsymbol{\pi}}\times\vec{\boldsymbol{\alpha}}\right)\psi \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\left(\psi^+\boldsymbol{\gamma}_5\psi\right) - c\nabla\cdot\left(\psi^+\vec{\boldsymbol{\Sigma}}\psi\right) = \dfrac{2m_\mathrm{e}c^2}{i\hbar}\psi^+\left(\boldsymbol{\gamma}_5\boldsymbol{\beta}\right)\psi \end{array}\right. , \qquad (19)$$

where as easily can be worked out

$$\vec{\boldsymbol{\alpha}}\otimes\vec{\boldsymbol{\Sigma}} = \begin{pmatrix} -\boldsymbol{\gamma}_5 & +i\alpha_\mathrm{z} & -i\alpha_\mathrm{y} \\ -i\alpha_\mathrm{z} & -\boldsymbol{\gamma}_5 & +i\alpha_\mathrm{x} \\ +i\alpha_\mathrm{y} & -i\alpha_\mathrm{x} & -\boldsymbol{\gamma}_5 \end{pmatrix}.$$

In order to identify in Equation (19), the role of the particle current density $\mathcal{J} = \psi^+ c\vec{\boldsymbol{\alpha}}\psi$ the following identities can be applied

$$\left\{\begin{array}{l} \nabla\cdot\left[\psi^+\left(\vec{\boldsymbol{\alpha}}\otimes\vec{\boldsymbol{\Sigma}}\right)\psi\right] = -i\nabla\times\left(\psi^+\vec{\boldsymbol{\alpha}}\psi\right) - \nabla\left(\psi^+\boldsymbol{\gamma}_5\psi\right) \\ \psi^+\left(\vec{\boldsymbol{\pi}}\times\vec{\boldsymbol{\alpha}}\right)\psi = i\hbar\psi^+\left(\vec{\boldsymbol{\alpha}}\times\nabla\right)\psi - e\vec{A}\times\left(\psi^+\vec{\boldsymbol{\alpha}}\psi\right) \end{array}\right. ,$$

such that Equation (19) is now of the form

$$\left\{\begin{array}{l} \dfrac{\mathrm{d}}{\mathrm{d}t}\left(\psi^+\vec{\boldsymbol{\Sigma}}\psi\right) - c\nabla\left(\psi^+\boldsymbol{\gamma}_5\psi\right) - i\,\nabla\times\vec{\mathcal{J}} = \dfrac{m_\mathrm{e}c}{\hbar}\psi^+\left(2\dfrac{\vec{\boldsymbol{\pi}}}{m_\mathrm{e}}\times\vec{\boldsymbol{\alpha}}\right)\psi \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\left(\psi^+\boldsymbol{\gamma}_5\psi\right) - c\nabla\cdot\left(\psi^+\vec{\boldsymbol{\Sigma}}\psi\right) = i\,\dfrac{m_\mathrm{e}c}{\hbar}\psi^+\left(2c\,\boldsymbol{\beta}\boldsymbol{\gamma}_5\right)\psi \end{array}\right. . \qquad (20)$$

Using $\overleftrightarrow{\mathcal{J}}^{(2)}$ from Equation (18) the latter reduces to the form given in [3]

$$\left\{\begin{array}{l} \dfrac{\mathrm{d}\vec{\mathcal{S}}}{\mathrm{d}t} - ic\,\nabla\mathcal{S}_4 = \dfrac{m_\mathrm{e}c}{\hbar}\vec{\mathcal{J}}_4^{(2)} + i\,\nabla\times\vec{\mathcal{J}} \\ i\,\dfrac{\mathrm{d}\mathcal{S}_4}{\mathrm{d}t} - c\nabla\cdot\vec{\mathcal{S}} = i\,\dfrac{m_\mathrm{e}c}{\hbar}\overleftrightarrow{\mathcal{J}}^{(2)} \end{array}\right. . \qquad (21)$$

It is important to note that despite the fact that the time evolution of the spin density has to be taken into account, the spin density *per se* has no well-defined physical meaning, since it does not refer to a constant of motion. It merely serves as an auxiliary quantity.

6. 'Vectorial' and 'tensorial' polarization particle current densities

Combining now Equation (16) with Equation (21) a closed set of differential equations is obtained that yields the time evolution of the polarization density in the presence of an external electromagnetic field:

$$\left\{\begin{array}{l} \dfrac{\mathrm{d}}{\mathrm{d}t}\vec{\mathcal{T}} + \nabla\cdot\left(\overleftrightarrow{\mathcal{J}}^{(1)} + \overleftrightarrow{\mathcal{J}}^{(2)}\right) = \dfrac{e}{m_{\mathrm{e}}}\left(\vec{\mathcal{S}}\times\vec{B} - \frac{1}{c}\,\vec{E}\,\mathcal{S}_4\right) \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{T}_4 + \nabla\cdot\left(\vec{\mathcal{J}}_4^{(1)} - \vec{\mathcal{J}}_4^{(2)}\right) = \dfrac{ie}{m_{\mathrm{e}}c}\vec{\mathcal{S}}\cdot\vec{E} \\ \dfrac{\mathrm{d}\vec{\mathcal{S}}}{\mathrm{d}t} - ic\nabla\mathcal{S}_4 = \dfrac{m_{\mathrm{e}}c}{\hbar}\vec{\mathcal{J}}_4^{(2)} + i\,\nabla\times\vec{\mathcal{J}} \\ i\,\dfrac{\mathrm{d}\mathcal{S}_4}{\mathrm{d}t} - c\nabla\cdot\vec{\mathcal{S}} = i\,\dfrac{m_{\mathrm{e}}c}{\hbar}\overleftrightarrow{\mathcal{J}}^{(2)} \end{array}\right. . \qquad (22)$$

In Equation (22), the scalar product symbol in $\nabla\cdot\overleftrightarrow{\mathcal{J}}^{(1)}$ has to be understood in the following way

$$\nabla\cdot\overleftrightarrow{\mathcal{J}}^{(1)} = \nabla\cdot\,\psi^{+}\left(\vec{T}\otimes\vec{\boldsymbol{\alpha}}\right)\psi = \Theta_{\mathrm{x}} + \Theta_{\mathrm{y}} + \Theta_{\mathrm{z}},$$

where

$$\Theta_{\nu} = \sum_{\mu}\partial_{\mu}\left[\psi^{+}\left(T_{\nu}\alpha_{\mu}\right)\psi\right].$$

Furthermore, since $\boldsymbol{\gamma}_5$ and $\boldsymbol{\beta}\boldsymbol{\gamma}_5$ are simple matrices and the Kronecker product for $\vec{\mathcal{J}}_4^{(2)}$ in Equation (18) is defined in a similar manner to that in Equation (14), namely as

$$\frac{\vec{\boldsymbol{\pi}}}{m_{\mathrm{e}}c}\times\vec{\boldsymbol{\alpha}} = \frac{1}{m_{\mathrm{e}}c}\begin{pmatrix} \pi_{\mathrm{x}}\alpha_{\mathrm{x}} & \pi_{\mathrm{x}}\alpha_{\mathrm{y}} & \pi_{\mathrm{x}}\alpha_{\mathrm{z}} \\ \pi_{\mathrm{y}}\alpha_{\mathrm{x}} & \pi_{\mathrm{y}}\alpha_{\mathrm{x}}\alpha_{\mathrm{y}} & \pi_{\mathrm{y}}\alpha_{\mathrm{x}}\alpha_{\mathrm{z}} \\ \pi_{\mathrm{z}}\alpha_{\mathrm{x}} & \pi_{\mathrm{z}}\alpha_{\mathrm{y}} & \pi_{\mathrm{z}}\alpha_{\mathrm{z}} \end{pmatrix}.$$

$\nabla\cdot\vec{\mathcal{J}}_4^{(2)}$ is therefore given by

$$\nabla\cdot\vec{\mathcal{J}}_4^{(2)} = c\nabla\cdot\,\psi^{+}\left(\frac{\vec{\boldsymbol{\pi}}}{m_{\mathrm{e}}c}\times\vec{\boldsymbol{\alpha}}\right)\psi = c\left(\Xi_{\mathrm{x}} + \Xi_{\mathrm{y}} + \Xi_{\mathrm{z}}\right),$$

where

$$\Xi_{\nu} = \sum_{\mu}\partial_{\mu}\left[\psi^{+}\left(\frac{\pi_{\nu}}{m_{\mathrm{e}}c}\alpha_{\mu}\right)\psi\right],$$

and the meaning of the term $\nabla\cdot\vec{\mathcal{S}} = \partial_{\mathrm{x}}\Sigma_{\mathrm{x}} + \partial_{\mathrm{y}}\Sigma_{\mathrm{y}} + \partial_{\mathrm{z}}\Sigma_{\mathrm{z}}$ follows from using a scalar product notation.

Fortunately, by means of Table 2 the remaining unfamiliar looking term in Equation (18) can be reformulated such that

$$T_4\vec{\boldsymbol{\alpha}} = -i\,\boldsymbol{\gamma}_5\left(\vec{\boldsymbol{\Sigma}}\cdot\frac{\vec{\boldsymbol{\pi}}}{m_{\mathrm{e}}c}\right)\vec{\boldsymbol{\Sigma}},$$

i.e. yields a sum of four-vectors of the type

$$T_4\alpha_{\nu} = \left(\Sigma_x\frac{\pi_x}{m_{\mathrm{e}}c}\right)\Sigma_{\nu} + \left(\Sigma_y\frac{\pi_y}{m_{\mathrm{e}}c}\right)\Sigma_{\nu} + \left(\Sigma_z\frac{\pi_z}{m_{\mathrm{e}}c}\right)\Sigma_{\nu}.$$

$\overleftrightarrow{\mathcal{J}}$ and $\vec{\mathcal{J}}_4$ can be interpreted as ***tensor** and **vector** polarization particle current densities,* and of course $\vec{\mathcal{J}} = \psi^+ \left(c\vec{\boldsymbol{\alpha}}\right) \psi$ is the well-known relativistic *particle current density.* Obviously, the time evolution of the polarization density is governed by the 'divergences' of these densities and by the interaction of the spin density $\mathcal{S}$ with the external electromagnetic field.

7. Time evolution of the magnetization density

Per definition the magnetization density $\vec{\mathcal{M}}_{\mathrm{e}}(\vec{r}, t)$, i.e. the relativistic spin magnetic moment density per unit volume of the electron in its own frame, is given by [9]

$$\vec{\mathcal{M}}_{\mathrm{e}}(\vec{r}, t) = \mu_{\mathrm{B}} \psi^+ (\vec{r}, t) \left(\boldsymbol{\beta} \vec{\boldsymbol{\Sigma}}\right) \psi(\vec{r}, t),$$

where μ_{B} is the Bohr magneton. Since the magnetization operator

$$\vec{M}_{\mathrm{e}} = \mu_{\mathrm{B}}\, \boldsymbol{\beta} \vec{\boldsymbol{\Sigma}}$$

is time independent, the time evolution of its density contains only two terms, namely

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\psi^+(\vec{r}, t)\, \vec{M}_{\mathrm{e}} \psi(\vec{r}, t)\right] = \frac{\partial \psi^+(\vec{r}, t)}{\partial t} \vec{M}_{\mathrm{e}} \psi(\vec{r}, t) + \psi^+(\vec{r}, t)\, \vec{M}_{\mathrm{e}} \frac{\partial \psi(\vec{r}, t)}{\partial t}\,.$$

With Hermitian scalar and vector potentials and by omitting the argument $(\vec{r}, t)$ one immediately gets

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\left(\psi^+ \vec{M}_{\mathrm{e}} \psi\right) = 2c\mu_{\mathrm{B}}\, \psi^+ \left(\boldsymbol{\gamma}_5 \boldsymbol{\beta} \vec{\pi}\right) \psi + c\psi^+ \left[\left(\vec{\boldsymbol{\alpha}} \cdot \vec{\boldsymbol{\pi}} - \vec{\boldsymbol{\pi}}^+ \cdot \vec{\boldsymbol{\alpha}}\right) \vec{M}_{\mathrm{e}}\right] \psi,$$

which reformulated yields

$$\frac{\mathrm{d}}{\mathrm{d}t} \vec{\mathcal{M}}_{\mathrm{e}} + c\, \nabla \cdot \left[\psi^+ \left(\vec{\boldsymbol{\alpha}} \otimes \vec{M}_{\mathrm{e}}\right) \psi\right] = \frac{iec}{m_{\mathrm{e}}} \psi^+ \left(\vec{\boldsymbol{\pi}} \boldsymbol{\beta} \boldsymbol{\gamma}_5\right) \psi, \tag{23}$$

where

$$\vec{\boldsymbol{\alpha}} \otimes \vec{M}_{\mathrm{e}} = \left(\vec{\boldsymbol{\Sigma}} \otimes \vec{M}_{\mathrm{e}}\right) \boldsymbol{\gamma}_5 = \mu_{\mathrm{B}} \boldsymbol{\beta} \left(\vec{\boldsymbol{\Sigma}} \otimes \vec{\boldsymbol{\Sigma}}\right) \boldsymbol{\gamma}_5\,. \tag{24}$$

On the rhs of Equation (23), $\psi^+ \left(\vec{\boldsymbol{\pi}} \boldsymbol{\beta} \boldsymbol{\gamma}_5\right) \psi$ is a kind of generalized moment density, since

$$\boldsymbol{\beta} \boldsymbol{\gamma}_5 = \begin{pmatrix} 0 & -\mathbf{I}_2 \\ \mathbf{I}_2 & 0 \end{pmatrix}.$$

As can be seen, in contrast to the time evolution of the polarization density, no terms with $\vec{B}$ and $\vec{E}$ occur in the time evolution of the magnetization density.

8. Bispinor representations and the non-relativistic limit

8.1. *The Pauli equation in the presence of an external electromagnetic field*

As is probably well known in viewing ψ in the time-dependent Dirac equation, Equations (2) and (9) as a bispinor [10]

$$\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}, \tag{25}$$

where ϕ and χ satisfy the following differential equations:

$$i\hbar\frac{\partial\phi}{\partial t} = c\vec{\boldsymbol{\pi}}\cdot\vec{\boldsymbol{\sigma}}\chi + \left(eV + m_{\mathrm{e}}c^2\right)\phi\,, \tag{26}$$

$$\chi = \frac{\vec{\boldsymbol{\pi}}\cdot\vec{\boldsymbol{\sigma}}}{2m_{\mathrm{e}}c}\phi - \frac{1}{2m_{\mathrm{e}}c^2}\left(i\hbar\frac{\partial}{\partial t} - eV - m_{\mathrm{e}}c^2\right)\chi\,, \tag{27}$$

with $\vec{\boldsymbol{\pi}} = (\vec{p} - e\vec{A})\mathbf{I}_2$. To lowest order (c^{-1}) χ is given [11,12] by

$$\chi^{(1)} = \frac{\vec{\boldsymbol{\pi}}\cdot\vec{\boldsymbol{\sigma}}}{2m_{\mathrm{e}}c}\phi, \tag{28}$$

which applied [13] on the rhs of Equation (27) leads to an expression for χ in terms of ϕ,

$$\chi^{(2)} = \left[1 - \frac{1}{2m_{\mathrm{e}}c^2}\left(i\hbar\frac{\partial}{\partial t} - eV - m_{\mathrm{e}}c^2\right)\right]\frac{\vec{\boldsymbol{\pi}}\cdot\vec{\boldsymbol{\sigma}}}{2m_{\mathrm{e}}c}\phi,$$

that in turn can be used in Equation (26) to yield a Pauli equation for ϕ with relativistic corrections up to the order of c^{-2}, [14]

$$\begin{aligned} i\hbar\frac{\partial\phi}{\partial t} &= \left(\frac{\vec{\boldsymbol{\pi}}^2}{2m_{\mathrm{e}}} - \mu_{\mathrm{B}}\vec{\boldsymbol{\sigma}}\cdot\vec{B} + eV + m_{\mathrm{e}}c^2\right)\phi \\ &\quad - \left[\frac{\vec{\boldsymbol{\pi}}^4}{8m_{\mathrm{e}}^3c^2} + \frac{e\hbar}{4m_{\mathrm{e}}^2c^2}\vec{\boldsymbol{\sigma}}\cdot\left(\vec{E}\times\vec{\boldsymbol{\pi}}\right) + \frac{ie\hbar}{4m_{\mathrm{e}}^2c^2}\left(\vec{\boldsymbol{\pi}}\cdot\vec{E}\right)\right]\phi. \end{aligned} \tag{29}$$

In Equation (29), the second term on the rhs corresponds to the 'spin-orbit' interaction and the third to the so-called Darwin term.

8.2. *Bispinor forms of the polarization, spin and magnetization densities and their time evolutions*

In terms of the bispinor representation Equation (25), the polarization and spin densities are then defined by

$$\begin{cases} \vec{\mathcal{T}} = \phi^+\vec{\boldsymbol{\sigma}}\phi - \chi^+\vec{\boldsymbol{\sigma}}\chi + \phi^+\dfrac{\vec{\boldsymbol{\pi}}}{m_{\mathrm{e}}c}\chi + \chi^+\dfrac{\vec{\boldsymbol{\pi}}}{m_{\mathrm{e}}c}\phi \\ \mathcal{T}_4 = \phi^+\left(\vec{\boldsymbol{\sigma}}\cdot\dfrac{\vec{\boldsymbol{\pi}}}{m_{\mathrm{e}}c}\right)\phi + \chi^+\left(\vec{\boldsymbol{\sigma}}\cdot\dfrac{\vec{\boldsymbol{\pi}}}{m_{\mathrm{e}}c}\right)\chi \end{cases},$$

$$\begin{cases} \vec{\mathcal{S}} = \phi^+\vec{\boldsymbol{\sigma}}\phi + \chi^+\vec{\boldsymbol{\sigma}}\chi \\ \mathcal{S}_4 = i\,\left(\phi^+\chi + \chi^+\phi\right) \end{cases},$$

and the terms $\overleftrightarrow{\mathcal{J}}$ and $\vec{\mathcal{J}}_4$ are given now by

$$\begin{cases} \overleftrightarrow{\mathcal{J}} = \phi^+ \left(\vec{\boldsymbol{\sigma}} \otimes \dfrac{\vec{\boldsymbol{\pi}}}{m_e} \right) \phi + \chi^+ \left(\vec{\boldsymbol{\sigma}} \otimes \dfrac{\vec{\boldsymbol{\pi}}}{m_e} \right) \chi \\ \qquad - \; c\, \phi^+ \left(\vec{\boldsymbol{\sigma}} \otimes \vec{\boldsymbol{\sigma}} \right) \chi + c\, \chi^+ \left(\vec{\boldsymbol{\sigma}} \otimes \vec{\boldsymbol{\sigma}} \right) \phi \\ \\ \vec{\mathcal{J}}_4 = \phi^+ \left(i \dfrac{\vec{\boldsymbol{\pi}}}{m_e} \times \vec{\boldsymbol{\sigma}} + \dfrac{\vec{\boldsymbol{\pi}}}{m_e} \right) \chi \\ \qquad + \; \chi^+ \left(i \dfrac{\vec{\boldsymbol{\pi}}}{m_e} \times \vec{\boldsymbol{\sigma}} + \dfrac{\vec{\boldsymbol{\pi}}}{m_e} \right) \phi \end{cases},$$

where

$$\vec{\boldsymbol{\sigma}} \otimes \vec{\boldsymbol{\sigma}} = \begin{pmatrix} \mathbf{I}_2 & i\sigma_z & -i\sigma_y \\ -i\sigma_z & \mathbf{I}_2 & i\sigma_x \\ i\sigma_y & -i\sigma_x & \mathbf{I}_2 \end{pmatrix}.$$

In a similar manner, for the magnetization density one obtains

$$\vec{\mathcal{M}}_e = \mu_B \left[\phi^+ \vec{\boldsymbol{\sigma}} \phi - \chi^+ \vec{\boldsymbol{\sigma}} \chi \right].$$

Quite clearly, depending on what kind of approximation is made in Equation (27) a variety of different relativistic corrections for the time evolution of the various densities can be constructed with expressions that increase in complexity with the order of $1/c$ terms included.

8.3. *Non-relativistic limit*

The advantage of introducing a bispinor representation is that the non-relativistic limit of Equations (16), (21) and (23) can easily be read off because for $c = \infty$ in Equation (28) $\chi = 0$, one immediately gets

$$\vec{\mathcal{T}} \equiv \vec{\mathcal{S}} \equiv \frac{\vec{\mathcal{M}}_e}{\mu_B} = \phi^+ \vec{\boldsymbol{\sigma}} \phi,$$
$$\overleftrightarrow{\mathcal{J}} = \phi^+ \left(\vec{\boldsymbol{\sigma}} \otimes \frac{\vec{\boldsymbol{\pi}}}{m_e} \right) \phi, \; \mathcal{T}_4, \mathcal{S}_4, \vec{\mathcal{J}}_4 = 0.$$

Consequently, the time evolution of the polarization, spin and magnetization density reduces to

$$\begin{cases} \dfrac{d}{dt} \vec{\mathcal{T}} + \nabla \cdot \overleftrightarrow{\mathcal{J}} = \dfrac{e}{m_e} \vec{\mathcal{S}} \times \vec{B} \\ \dfrac{d}{dt} \vec{\mathcal{M}}_e + \nabla \cdot \left(\mu_B \overleftrightarrow{\mathcal{J}} \right) = \dfrac{e}{m_e} \vec{\mathcal{M}}_e \times \vec{B} \end{cases}. \tag{30}$$

Comparing now Equation (16) with its non-relativistic counterpart in Equation (30), one easily can see that in the latter case (a), the interaction with the electric field $\vec{E}$ is missing and (b) $\vec{\mathcal{S}}$ is reduced to a 2×2 matrix vector, since $\vec{\boldsymbol{\sigma}} = (\sigma_x, \sigma_y, \sigma_z)$. The term $\vec{\boldsymbol{\sigma}} \otimes \vec{\boldsymbol{\pi}}$ refers to a 3×3 supermatrix,

$$\vec{\boldsymbol{\sigma}} \otimes \vec{\boldsymbol{\pi}} = \begin{pmatrix} \sigma_x\pi_x & \sigma_x\pi_y & \sigma_x\pi_z \\ \sigma_y\pi_x & \sigma_y\pi_y & \sigma_x\pi_z \\ \sigma_z\pi_x & \sigma_z\pi_y & \sigma_x\pi_z \end{pmatrix}.$$

that now corresponds to a 6×6 square matrix. The 'divergence' of the tensorial particle current density $\nabla \cdot \overleftrightarrow{\mathcal{J}}$ in the non-relativistic case is then given by

$$\nabla \cdot \overleftrightarrow{\mathcal{J}} = \Theta_{\mathrm{x}} + \Theta_{\mathrm{y}} + \Theta_{\mathrm{z}}.$$

$$\Theta_\nu = \frac{1}{m_{\mathrm{e}}} \sum_\mu \partial_\mu \left[\psi^+ \left(\sigma_\nu \pi_\mu\right) \psi\right].$$

As already mentioned in the introduction, it is important to point out that in all non-relativistic interpretations of experiments, in which an external electric field is applied, the time evolution of the polarization density is independent of $\vec{E}$. Furthermore, because of the SU2 invariance of the Pauli matrices for $\vec{\mathcal{S}}$ and $\vec{\mathcal{M}}_{\mathrm{e}} = \mu_{\mathrm{B}} \vec{\mathcal{S}}$ no preferred direction can be defined.

9. Further considerations

Quite clearly, up-to-now only the case of a single electron was considered. Suppose that as proposed in [5], the single-electron Dirac operator in Equation (2) can be replaced by an effective Dirac operator

$$\mathcal{H}_{eff}(\vec{r}, t) = T + V_{eff}(\vec{r}, t; [n(\vec{r}, t)]),$$

where T is the single particle kinetic energy operator and $V_{eff}(\vec{r}, t; [n(\vec{r}, t)])$ an effective potential of the form

$$\begin{aligned} V_{eff}(\vec{r}, t; [n(\vec{r}, t)]) = {} & V_{ext}(\vec{r}, t) + V_H(\vec{r}, t; [n(\vec{r}, t)]) \\ & + V_{xc}(\vec{r}, t; [n(\vec{r}, t)]). \end{aligned}$$

Of course such an assumption invokes immediately all the formal difficulties connected with the time-dependent density functional theory (TDFT) [15–19]. Assuming the simplest possible approximation [20], namely the so-called adiabatic local density approximation (ALDA) , the exchange-correlation potential $V_{xc}(\vec{r}, t; [n(\vec{r}, t), \vec{m}(\vec{r}; t)])$ and effective exchange field $\vec{B}(\vec{r}, t; [n(\mathbf{r}, t), \vec{m}(\vec{r}; t)])$ of an in general magnetic system are given by

$$V_{xc}(\vec{r}, t; [n(\vec{r}, t), \vec{m}(\vec{r}; t)]) = \frac{\delta E_{xc}[n(\vec{r}; t), \vec{m}(\vec{r}; t)]}{\delta n(\vec{r}; t)},$$

$$\vec{B}(\vec{r}, t; [n(\vec{r}, t), \vec{m}(\vec{r}; t)]) = \frac{e\hbar}{2mc} \frac{\delta E_{xc}[n(\vec{r}; t), \vec{m}(\vec{r}; t)]}{\delta \vec{m}(\vec{r}; t)}, \tag{31}$$

where $n(\vec{r}, t) \equiv n$ and $\vec{m}(\vec{r}; t) \equiv \vec{\mathcal{M}}_{\mathrm{e}}$ are the particle and magnetization density, respectively.

Since all densities to be considered are of bilinear form, it was suggested [5] to describe their time dependence in terms of instantaneous resolvents $G(z, t)$ of $\mathcal{H}_{eff}(\vec{r}, t)$, an approach that deals with time dependency (at least) on the level of first-order time-dependent perturbation theory. Imposing particle conservation, this implies

$$\frac{\delta\omega(\vec{r};t)}{\delta t} \simeq -\pi^{-1}\left\{ \mathrm{Im}Tr \int\limits_{E_b(t)}^{E_F(t)} \langle\vec{r}|\,\mathbb{O}\frac{\delta G(z;t)}{\delta t}\,|\vec{r}\rangle\,\mathrm{d}z \right.$$
$$\left. + \,\mathrm{Im}\,\langle\vec{r}|\,\mathbb{O}G\left(E_F\left(t\right);t\right)|\vec{r}\rangle \right\}, \tag{32}$$

where $E_b(t)$ and $E_F(t)$ are the band bottom and the Fermi energy. The operator $\mathbb{O}$ and the corresponding density $\omega(\vec{r};t)$ in Equation (32) can be picked up from Table 3. In principle, if needed also the time evolution of the tensorial and vector current probabilities in Equation (18) can approximately be determined.

One particular aspect has to be mentioned in the context of using LDA: because of the non-relativistic origin of the usually applied local DFT parametrizations: $\vec{B}\left[n,\vec{\mathcal{M}}_{\mathrm{e}}\right]$ in Equation (31) is only defined along an arbitrary z-direction, which in turn implies that instead of $\vec{\boldsymbol{\Sigma}}$ it is sufficient to consider only Σ_z. Orientations other than along the z-direction can only be introduced by similarity transformations of $\mathcal{H}_{eff}(\vec{r},t)$, see e.g. [21].

10. Conclusion

In the last few years, fully relativistic *ab initio* schemes were frequently applied to describe typical spintronic properties such as, e.g. the change in resistivity of realistic nanosystems with respect to the orientation of the magnetic field.[22] Even attempts were made to determine switching times and critical currents by means of multi-scale approaches using the LLG equation and other 'classical' relations with ab initio parameters. The obtained results agreed reasonably well [23] with the corresponding experimental data and suggested that in dealing theoretically with time-dependent properties this leads to completely new insights of switching processes [24]. However, in all these multi-scale schemes, a correct description of time dependence was only circumvented.

It was the purpose of this paper to give a consistent derivation of the time evolution of the polarization, spin and magnetization densities in terms of the time-dependent Dirac equation and to compare these densities with their non-relativistic counterparts. Furthermore, in order to at least indicate what numerical procedures could be used to approximate these time evolutions in the case of realistic solid systems, the method of instantaneous resolvents as discussed in [5] was recalled.

Quite clearly, there are still a lot of formal difficulties piled up on the way to a proper theoretical description of changes in physical properties on a short time scale. However, one has to realize that with the arrival of nanophysics no longer further (useful) reductions in length scales can be expected. In future, only time scales can further be reduced. The present paper is meant to contribute to the understanding of time-dependent phenomena.

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