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Spin–orbit coupling in the spin-current-density-functional theory

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Abstract

Starting from the spin-current-density-functional theory for electronic systems, we extend the formulation to include spin–orbit coupling. Particular attention is devoted to the symmetry of the problem. Here we show that the exchange-correlation energy functional is invariant by the $U(1)_{\rm em} \times SU(2)_{\rm spin}$ gauge transformations. We give the transformation laws of the paramagnetic current and also the paramagnetic spin current density by the $U(1)_{\rm em} \times SU(2)_{\rm spin}$ gauge transformations. For the case where the spin–orbit coupling is taken into account, we generalize the equations of continuity satisfied by the current density and the spin current density, derived by Vignale and Rasolt.

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1. Introduction

The density functional theory (DFT) is a theory of electronic structure [1–3] which uses the electron density distribution $n(\mathbf{r})$ as a basic variable, instead of the many-electron wavefunction $\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$. For systems subject to external magnetic fields, currents are induced. It is then practical to use a DFT which employs the current density. The basic theory for this current-density-functional theory (CDFT) has been developed by Vignale and Rasolt [4] (in the following abbreviated as VR). As shown by VR the basic variables are now the electron density $n(\mathbf{r})$ and the paramagnetic current density $\mathbf{j}_p(\mathbf{r})$ (see the next section for definitions). The total energy $E(n, \mathbf{j}_p)$ is now a functional of the $n, \mathbf{j}_p$ densities. The VR formalism of the CDFT can be summarized as follows:

(i) They have demonstrated the gauge invariance of the exchange-correlation (xc) energy functional by the $U(1)_{\rm em}$ gauge transformation. This leads to a formulation of the theory in terms of the $U(1)_{\rm em}$ gauge invariant vorticity vector $\boldsymbol{\nu} = \boldsymbol{\nabla} \times (\mathbf{j}_p/n)$.
(ii) They have given the specific form of the one-particle Kohn–Sham (KS) equation which is $U(1)_{\rm em}$ gauge invariant.

Extending these findings of CDFT to include the spin-degrees of freedom, VR formulate the spin current DFT (SCDFT) [5]. For the general case where the electrons are subjected to a magnetic field with an arbitrary direction, the authors have shown that one has to add to the previous $n, \mathbf{j}_p$ densities two other quantities for a complete description of the system: the spin vector density $\mathbf{s}(\mathbf{r})$ and the paramagnetic spin current vector densities $\mathbf{J}_{p\lambda=1,2,3}(\mathbf{r})$. Hence, one should consider the total energy as a functional of the set of densities $(n, \mathbf{j}_p, \mathbf{s}, \mathbf{J}_{p\lambda})$, i.e., $E(n, \mathbf{j}_p, \mathbf{s}, \mathbf{J}_{p\lambda})$.

The main purpose of the present paper is to generalize the VR formalism of SCDFT by including the spin–orbit coupling (SOC). In section 2, it will be shown how to include such a relativistic effect from the usual SCDFT. We shall give the many-body Hamiltonian, then we will derive the corresponding Pauli-like one-electron equation. The second part of section 2 is devoted to the symmetry aspects of the problem in the presence of the SOC. Taking stock of the study performed in [6], it will be shown that the theory of SCDFT with SOC exhibits a local $U(1)_{\rm em} \times SU(2)_{\rm spin}$ gauge invariance which leads to a gauge invariant xc energy functional. We shall present in section 3 the $U(1)_{\rm em} \times SU(2)_{\rm spin}$ gauge transformation laws of the current densities $\mathbf{j}_p$ and $\mathbf{J}_{p\lambda}$. The transformation laws given by equations (6.14) in [5] and also equations (6.4) in [8] are only valid for an infinitesimal local spin rotation [9]; here the generalized expressions will be derived for a finite local spin transformation. These expressions reduce to those obtained by VR for the particular case of an infinitesimal local spin rotation. Finally, in section 4, we will derive the equation of continuity satisfied by the paramagnetic current density $\mathbf{j}_p$ and also the modified equation of continuity satisfied by the paramagnetic spin current density $\mathbf{J}_{p\lambda}$. Such equations contain terms arising from SOC. A summary of the main results will be given in section 5.

2. Spin–orbit coupling in the spin current DFT

In this section, we show explicitly how the ground-state (gs) energy functional of an N-electron system, subjected to a static electromagnetic field ($\mathbf{E} = -\nabla V, \mathbf{B} = \nabla \times \mathbf{A}$), can be written in terms of the SOC term. In the rest of the paper, the spin indices are labelled by σ, σ'. The Hamiltonian of SCDFT is given by [5]

$$H^{op} = \sum_{j=1}^{N} \frac{1}{2m}\left[\mathbf{p}_j + \frac{e}{c}\mathbf{A}(\mathbf{r}_j)\right]^2 + \frac{1}{2}\sum_{\substack{i,j \\ i\neq j}}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \int \mathrm{d}^3 r\, n^{op}(\mathbf{r}) V(\mathbf{r}) + \frac{e\hbar}{2mc}\int \mathrm{d}^3 r\, \mathbf{s}^{op}(\mathbf{r}) \cdot \mathbf{B} \tag{1}$$

where $\mathbf{r}_j$ and $\mathbf{p}_j = \frac{\hbar}{\mathrm{i}}\nabla_j$ are the coordinate and momentum operators of the jth electron. The particle density is defined in terms of the field operators $\Psi_\sigma(\mathbf{r})$ by

$$n(\mathbf{r}) = \langle n^{op}(\mathbf{r})\rangle = \sum_{\sigma} \left\langle \Psi_\sigma^+(\mathbf{r})\Psi_\sigma(\mathbf{r})\right\rangle \tag{2}$$

where $\langle\rangle$ means the gs expectation value. The spin vector density is

$$\mathbf{s}(\mathbf{r}) = \sum_{\sigma\sigma'} \left\langle \Psi_\sigma^+(\mathbf{r})\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle\Psi_{\sigma'}(\mathbf{r})\right\rangle \tag{3}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ stands for the vector of 2×2 Pauli matrices. Generally, the many-body

Hamiltonian is written in terms of the paramagnetic current density as

$$H^{op} = \sum_{j=1}^{N} \frac{1}{2m}\mathbf{p}_j^2 + \frac{1}{2}\sum_{\substack{i,j \\ i\neq j}}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{e}{c}\int \mathrm{d}^3 r\, \mathbf{j}_p^{op}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r}) + \frac{e^2}{2mc^2}\int \mathrm{d}^3 r\, n^{op}(\mathbf{r})\mathbf{A}^2(\mathbf{r}) + \int \mathrm{d}^3 r\, V(\mathbf{r}) n^{op}(\mathbf{r}) + \frac{e\hbar}{2mc}\int \mathrm{d}^3 r\, \mathbf{s}^{op}(\mathbf{r})\cdot\mathbf{B} \quad (4)$$

where the paramagnetic current density, $\mathbf{j}_p(\mathbf{r})$, is defined as the gs expectation value of the operator $\mathbf{j}_p^{op}(\mathbf{r}) = (\hbar/2m\mathrm{i})\sum_\sigma \left[\Psi_\sigma^+(\mathbf{r})(\nabla\Psi_\sigma(\mathbf{r})) - \left(\nabla\Psi_\sigma^+(\mathbf{r})\right)\Psi_\sigma(\mathbf{r})\right]$.

We now state the VR formalism by including the SOC term. The SOC being a relativistic effect, one formally should start with the Dirac equation. To obtain the correct SOC term, one has to expand the Dirac equation up to the second order in $1/m$ by using the well-known Foldy–Wouthuyson scheme. To introduce the SOC term in the nonrelativistic Hamiltonian one can follow the scheme proposed in [7], which consists in simply substituting in the kinetic energy term, equation (1), the canonical momentum operator $\mathbf{\Pi} = \mathbf{p} + (e/c)\mathbf{A}$ by $\mathbf{\Pi} = \mathbf{p} + (e/c)\mathbf{A} + (e\hbar/4mc^2)(\boldsymbol{\sigma}\times\mathbf{E})$. Doing this substitution the Hamiltonian can then be written as

$$H^{op} = \sum_{j=1}^{N} \frac{1}{2m}\left[\mathbf{p}_j + \frac{e}{c}\mathbf{A}(\mathbf{r}_j) + \frac{e\hbar}{4mc^2}(\boldsymbol{\sigma}\times\mathbf{E})\right]^2 + \frac{1}{2}\sum_{\substack{i,j \\ i\neq j}}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \times \int \mathrm{d}^3 r\, V(\mathbf{r}) n^{op}(\mathbf{r}) + \frac{e\hbar}{2mc}\int \mathrm{d}^3 r\, \mathbf{s}^{op}(\mathbf{r})\cdot\mathbf{B}. \quad (5)$$

Note that all relativistic terms different from the spin–orbit coupling are ignored. In the subsequent analysis, it turns out to be more convenient to rewrite the term $(e\hbar/4mc^2)(\boldsymbol{\sigma}\times\mathbf{E})$ as

$$\frac{e\hbar}{4mc^2}(\boldsymbol{\sigma}\times\mathbf{E}) = \frac{e}{c}\sum_{\lambda=1}^{3}\mathbf{A}_\lambda\sigma_\lambda \quad (6)$$

where the set of three vector fields $(\mathbf{A}_1,\ \mathbf{A}_2,\ \mathbf{A}_3)$ is defined through the above equation from which we get a relationship between $\mathbf{A}_{\lambda=1,2,3}$ and the external electric field $\mathbf{E}$:

$$\mathbf{A}_\lambda(\mathbf{r}) = \frac{\hbar}{4mc}\sum_{\mu=1}^{3}\sum_{\nu=1}^{3}\epsilon_{\mu\lambda\nu}\mathbf{e}_\mu E_\nu \qquad E_\lambda = \frac{2mc}{\hbar}\sum_{\mu=1}^{3}\sum_{\nu=1}^{3}\epsilon_{\lambda\mu\nu}(\mathbf{e}_\mu\cdot\mathbf{A}_\nu) \quad (7)$$

where $\mathbf{e}_\mu$ denotes the unit vector of the physical space and E_ν is the νth component of the external electric field $\mathbf{E}$. Note that the term appearing on the right-hand side of equation (6) is just another way of writing the spin–orbit term. This form was adopted in [6] and is convenient for writing the equations of continuity as will be shown in section 4.

Let us now write down the total energy functional of the system. Following the Kohn–Sham scheme [2], we assume that the true densities are reproducible from orbitals of a noninteracting system [5]. Let $|\Phi\rangle$ stand for the ground-state wavefunction of the latter fictitious noninteracting N-electron system. By definition $|\Phi\rangle$ is a Slater determinant of N-one-electron two-spinor state $|\psi_j\rangle$. Thus, the total energy functional is given by

$$E = \sum_{j=1}^{N}\langle\psi_j|\frac{1}{2m}\left[\mathbf{p} + \frac{e}{c}\mathbf{A} + \frac{e}{c}\sum_{\lambda=1}^{3}\mathbf{A}_\lambda\sigma_\lambda\right]^2|\psi_j\rangle + E_{\mathrm{Hartree}} + \int \mathrm{d}^3 r\, V(\mathbf{r}) n(\mathbf{r}) + \frac{e\hbar}{2mc}\int \mathrm{d}^3 r\, \mathbf{s}(\mathbf{r})\cdot\mathbf{B} + E_{\mathrm{xc}} \quad (8)$$

where $E_{\rm Hartree}$ and $E_{\rm xc}$ are the Hartree and the xc energy functionals, respectively. To show explicitly the functional dependence of the total energy E on the various densities, we should expand the first term on the right-hand side of the above equation. Since the SOC is taken into account, one has to add the paramagnetic spin current density $\mathbf{J}_{p\lambda=1,2,3}(\mathbf{r})$ [5], which is the gs expectation value of $\mathbf{J}^{op}_{p\lambda}(\mathbf{r}) = (\hbar/2m\mathrm{i})\sum_{\sigma\sigma'}\left\{\Psi^{+}_{\sigma}(\nabla\Psi_{\sigma'}) - \left(\nabla\Psi^{+}_{\sigma}\right)\Psi_{\sigma'}\right\}\langle\sigma|\boldsymbol{\sigma}_{\lambda}|\sigma'\rangle$. Therefore the total energy can be written in the form

$$\begin{aligned} E(n,\mathbf{j}_p,\mathbf{s},\mathbf{J}_{p\lambda}) &= T_s(n,\mathbf{j}_p,\mathbf{s},\mathbf{J}_{p\lambda}) + E_{\rm Hartree} + E_{\rm xc}(n,\mathbf{j}_p,\mathbf{s},\mathbf{J}_{p\lambda}) \\ &+ \int \mathrm{d}^3r\, nV + \frac{e}{c}\int \mathrm{d}^3r\, \mathbf{j}_p\cdot\mathbf{A} + \frac{e}{c}\sum_{\lambda=1}^{3}\int \mathrm{d}^3r\, \mathbf{J}_{p\lambda}\cdot\mathbf{A}_{\lambda} \\ &+ \frac{e^2}{2mc^2}\int \mathrm{d}^3r\, n\mathbf{A}^2 + \frac{e^2}{2mc^2}\sum_{\lambda=1}^{3}\int \mathrm{d}^3r\, n\mathbf{A}_{\lambda}^2 \\ &+ \frac{e^2}{mc^2}\sum_{\lambda=1}^{3}\int \mathrm{d}^3r\, \mathbf{A}\cdot\mathbf{A}_{\lambda}s_{\lambda} + \frac{e\hbar}{2mc}\int \mathrm{d}^3r\, \mathbf{s}\cdot\mathbf{B} \end{aligned} \tag{9}$$

where $T_s = \sum_{j=1}^{N}\langle\psi_j|\frac{1}{2m}\left(\frac{\hbar}{\mathrm{i}}\nabla\right)^2|\psi_j\rangle$ is the noninteracting kinetic energy functional and $s_{\lambda}(\mathbf{r})$ is the λth component of the spin density $\mathbf{s}(\mathbf{r})$. In equation (9), we emphasize the fact that T_s, $E_{\rm xc}$ and E depend now on the set of densities $(n,\mathbf{j}_p,\mathbf{s},\mathbf{J}_{p\lambda})$.

Now, one can derive the Pauli-like equation by the minimization of the total energy functional with respect to $|\psi_j\rangle$. It turns out to be more convenient not to choose equation (9), but rather to choose equation (8) for the variational procedure. This yields the following equation:

$$\begin{aligned} \left[\frac{1}{2m}\left(\mathbf{p} + \frac{e}{c}\mathbf{A} + \frac{e}{c}\sum_{\lambda=1}^{3}\mathbf{A}_{\lambda}\sigma_{\lambda}\right)^2 + U^{\rm eff} + \frac{e}{2mc}\left(\mathbf{p}\cdot\left(\mathbf{A}_{\rm xc} + \sum_{\lambda=1}^{3}\mathbf{A}_{{\rm xc}\lambda}\sigma_{\lambda}\right)\right.\right. \\ \left.\left. + \left(\mathbf{A}_{\rm xc} + \sum_{\lambda=1}^{3}\mathbf{A}_{{\rm xc}\lambda}\sigma_{\lambda}\right)\cdot\mathbf{p}\right)\right]|\psi_j\rangle = \varepsilon_j|\psi_j\rangle \end{aligned} \tag{10}$$

where the spin-dependent effective scalar potential, $U^{\rm eff}$, is given by

$$U^{\rm eff} = e^2\int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}^3r' + V + V_{\rm xc} + (\mathbf{V}+\mathbf{V}_{\rm xc})\cdot\sigma \tag{11}$$

with $\mathbf{V} = (e\hbar/2mc)\mathbf{B}$. Moreover, the various xc potentials are defined as functional derivatives of $E_{\rm xc}(n,\mathbf{j}_p,\mathbf{s},\mathbf{J}_{p\lambda})$, i.e.

$$V_{\rm xc} = \frac{\delta E_{\rm xc}(n,\mathbf{j}_p,\mathbf{s},\mathbf{J}_{p\lambda})}{\delta n} \tag{12}$$

$$\mathbf{V}_{\rm xc} = \frac{\delta E_{\rm xc}(n,\mathbf{j}_p,\mathbf{s},\mathbf{J}_{p\lambda})}{\delta \mathbf{s}} \tag{13}$$

$$\frac{e}{c}\mathbf{A}_{\rm xc} = \frac{\delta E_{\rm xc}(n,\mathbf{j}_p,\mathbf{s},\mathbf{J}_{p\lambda})}{\delta \mathbf{j}_p} \tag{14}$$

$$\frac{e}{c}\mathbf{A}_{{\rm xc}\lambda} = \frac{\delta E_{\rm xc}(n,\mathbf{j}_p,\mathbf{s},\mathbf{J}_{p\lambda})}{\delta \mathbf{J}_{p\lambda}} \qquad \lambda = 1,2,3. \tag{15}$$

Finally, equation (10) can also be rewritten in the form

$$\left[\frac{1}{2m}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}^{\mathrm{eff}}\right)^2+U^{\mathrm{eff}}+\frac{e^2}{2mc^2}\left(\mathbf{A}^2+\sum_{\lambda=1}^{3}\mathbf{A}_\lambda^2+\mathbf{2}\sum_{\lambda=1}^{3}\mathbf{A}\cdot\mathbf{A}_\lambda\sigma_\lambda-(\mathbf{A}^{\mathrm{eff}})^2\right)\right]|\psi_j\rangle = \varepsilon_j|\psi_j\rangle. \tag{16}$$

Here the spin-dependent effective vector potential $\mathbf{A}^{\mathrm{eff}}$ is defined as

$$\mathbf{A}^{\mathrm{eff}}=\mathbf{A}+\mathbf{A}_{\mathrm{xc}}+\sum_{\lambda=1}^{3}(\mathbf{A}_\lambda+\mathbf{A}_{\mathrm{xc}\lambda})\sigma_\lambda. \tag{17}$$

Equation (16) is similar to equation (6.4) of [5] obtained by VR in SCDFT for the case where the magnetic field has an arbitrary direction. However, in [5] the terms depending on $\mathbf{A}_{\lambda=1,2,3}$ are not present. In fact these potential vectors, introduced in [5] (equation (6.3b)), were merely regarded as a mathematical convenience and were set equal to zero. In the present formalism, it is shown that these terms describe, in fact, the spin–orbit coupling and are related to the external electric field.

In the remainder of this section, we propose to focus on the gauge symmetry of SCDFT in the presence of the SOC term. This symmetry will be investigated in a somewhat different way, along the lines of [6]. Before proceeding, it is useful to recall that VR used the gauge symmetry in the SCDFT for the case where the external magnetic field has a constant $\hat{z}$ direction. As stated in the introduction, they proved the covariance of the one-electron equation and found the important result that $E_{\mathrm{xc}}(n,\mathbf{j}_p)$ is gauge invariant. When generalizing SCDFT to the case where the magnetic field is pointing in an arbitrary direction, VR introduced a more general symmetry which consists of a combined spin rotation and gauge transformation. They found that $E_{\mathrm{xc}}(n,\mathbf{j}_p,\mathbf{s},\mathbf{J}_{p\lambda})$ is invariant by such a symmetry. In the following, we consider the latter symmetry in our analysis of the SCDFT with SOC. Before going further, one may point out that the transformation given by equations (6.11) and (6.12) in [5] has not been explicitly recognized as being the time-independent $U(1)_{\mathrm{em}}\times SU(2)_{\mathrm{spin}}$ gauge transformation. Let us briefly recall some basics concerning the $U(1)_{\mathrm{em}}$ and $SU(2)_{\mathrm{spin}}$ transformation. In the following, any transformed quantity will be primed.

The $U(1)_{\mathrm{em}}$ acts on the wavefunction $|\psi_j\rangle$ by local phase transformation

$$\begin{aligned} &U(1)_{\mathrm{em}}:|\psi_j\rangle\rightarrow|\psi_j'\rangle=\exp\left[\frac{\mathrm{i}e}{\hbar c}\Lambda_0(\mathbf{r})\right]|\psi_j\rangle \\ &\mathbf{A}\rightarrow\mathbf{A}'=\mathbf{A}-\boldsymbol{\nabla}\Lambda_0(\mathbf{r}) \end{aligned} \tag{18}$$

where $\Lambda_0(\mathbf{r})$ is an arbitrary real-valued function and the non-Abelian $SU(2)_{\mathrm{spin}}$ transformation is defined as

$$SU(2)_{\mathrm{spin}}:\qquad |\psi_j\rangle\rightarrow|\psi_j'\rangle=U_S(\mathbf{r})\,|\psi_j\rangle. \tag{19}$$

Here $U_S(\mathbf{r})=\exp[(\mathrm{i}e/\hbar c)\Lambda(\mathbf{r})\cdot\boldsymbol{\sigma}]$ is a unitary local operator, with $\Lambda(\mathbf{r})$ an arbitrary position-dependent vector. Recall that the well-known expansion of the $U_S(\mathbf{r})$ is

$$U_S(\mathbf{r})=I\cos(\theta/2)+\mathrm{i}(\mathbf{u}\cdot\boldsymbol{\sigma})\sin(\theta/2) \tag{20}$$

with $\theta(\mathbf{r})=(2e/\hbar c)\,|\boldsymbol{\Lambda}(\mathbf{r})|$ and $\mathbf{u}=\boldsymbol{\Lambda}(\mathbf{r})/|\boldsymbol{\Lambda}(\mathbf{r})|$ a unit vector of arbitrary direction.

Let us now turn to the symmetry of SCDFT with SOC. Consider the expression of the total energy given by equation (8). Under the gauge transformations (equations (18) and (19)), the first term, namely $\sum_{j=1}^{N}\langle\psi_j|\frac{1}{2m}\left[\mathbf{p}+\frac{e}{c}\mathbf{A}(\mathbf{r})+\frac{e}{c}\sum_{\lambda=1}^{3}\mathbf{A}_\lambda(\mathbf{r})\sigma_\lambda\right]^2|\psi_j\rangle$, can be shown to be invariant, providing the term $\frac{e}{c}\sum_{\lambda=1}^{3}\mathbf{A}_\lambda\sigma_\lambda$ transforms according to the law

$$\frac{e}{c}\sum_{\lambda=1}^{3}\mathbf{A}_\lambda\sigma_\lambda\rightarrow\frac{e}{c}\sum_{\lambda=1}^{3}\mathbf{A}_\lambda'\sigma_\lambda=\frac{e}{c}\sum_{\lambda=1}^{3}\mathbf{A}_\lambda\left(U_S\sigma_\lambda U_S^{-1}\right)-\mathrm{i}\hbar\left(U_S\boldsymbol{\nabla}U_S^{-1}\right). \tag{21}$$

From equation (21), one obtains the transformation law for $\mathbf{A}_\lambda$:

$$\frac{e}{c}\mathbf{A}'_\lambda = \sum_{\mu=1}^{3} R_{\lambda\mu}(\theta)\left[\frac{e}{c}\mathbf{A}_\mu + \mathrm{i}\frac{\hbar}{2}\,\mathrm{Tr}_\sigma\left(\sigma_\mu U_S^{-1}\nabla U_S\right)\right] \tag{22}$$

where Tr_σ denotes the trace over the spin, and $R_{\lambda\mu}(\theta)$ are the matrix elements of the rotation operator $\mathbf{R}$ in physical space. Furthermore, the potential $\mathbf{V}(\mathbf{r})$ and the density $\mathbf{s}(\mathbf{r})$ experience the same rotation $\mathbf{R}$ under the gauge transformations [6]:

$$SU(2)_{\mathrm{spin}} : V_\lambda \rightarrow V'_\lambda = \sum_{\mu=1}^{3} R_{\lambda\mu}(\boldsymbol{\theta})V_\mu \tag{23}$$

$$s_\lambda \rightarrow s'_\lambda = \sum_{\mu=1}^{3} R_{\lambda\mu}(\boldsymbol{\theta})s_\mu. \tag{24}$$

Note that since $\mathbf{V}\cdot s = \mathbf{V}'\cdot\mathbf{s}'$, the fourth term on the right-hand side of equation (8) is gauge invariant. Moreover, the second and third terms are known to be invariant. Consequently, the fifth term (the xc energy E_{xc}) of equation (8) is gauge invariant since the total energy is invariant. Hence, the xc energy functional, E_{xc}, is invariant by $U(1)_{\mathrm{em}} \times SU(2)_{\mathrm{spin}}$ gauge transformations. It is important to stress that, if the vectors $\mathbf{A}_{\lambda=1,2,3}$ vanish (no spin–orbit coupling), the gauge symmetry ($SU(2)_{\mathrm{spin}}$) of the present formalism will be automatically broken. Indeed, this can be seen from equation (21). The transformation law of the vector $\frac{e}{c}\sum_{\lambda=1}^{3}\mathbf{A}_\lambda\sigma_\lambda$ is nontrivial; it contains an additional inhomogeneous term $\mathrm{i}\hbar\left(U_S\nabla U_S^{-1}\right)$ (see also equation (2.16) in [6]). In fact this particular term which arises from the action of the operator momentum $\mathbf{p} = \frac{\hbar}{\mathrm{i}}\nabla$ on the wavefunction in the expression of the total energy functional (8), cannot be eliminated in the absence of the term $\frac{e}{c}\sum_{\lambda=1}^{3}\mathbf{A}_\lambda\sigma_\lambda$. This important remark means that imposing a $U(1)_{\mathrm{em}}\times SU(2)_{\mathrm{spin}}$ gauge symmetry on the theory automatically induces the inclusion of the spin–orbit coupling. This result agrees with that reported by Fröhlich and Studer in [6]. Indeed, they showed that the one-particle quantum mechanics based on the Pauli equation exhibits a local $U(1)_{\mathrm{em}} \times SU(2)_{\mathrm{spin}}$ gauge invariance. They have established that the $SU(2)_{\mathrm{spin}}$ gauge fields consist of terms describing spin–orbit coupling.

As a final point related to $U(1)_{\mathrm{em}} \times SU(2)_{\mathrm{spin}}$ gauge symmetry, we briefly comment on the covariance of equation (16). Since the energy functional (8) is gauge invariant, the corresponding one-electron equation, equation (16), is automatically form invariant (covariant). Indeed, the covariance of equation (16) can be explicitly shown. We shall not make the derivation here but briefly indicate the main point. In order to achieve the derivation, one has to find the gauge transformation laws of the various xc potentials, V_{xc}, $\mathbf{V}_{\mathrm{xc}}$, $\mathbf{A}_{\mathrm{xc}}$ and $\mathbf{A}_{\mathrm{xc}\lambda}$. This point can be carried out by using the invariance of the xc energy functional, i.e.

$$E_{\mathrm{xc}}(n', \mathbf{j}'_p, \mathbf{s}', \mathbf{J}'_{p\lambda}) = E_{\mathrm{xc}}(n, \mathbf{j}_p, \mathbf{s}, \mathbf{J}_{p\lambda}). \tag{25}$$

These transformation laws can then be obtained by differentiating both sides of equation (25) with respect to n, $\mathbf{j}_p$, $\mathbf{s}$ and $\mathbf{J}_{p\lambda}$ and invoking the definitions of equations (12)–(15). Finally, note that in order to differentiate equation (25), we need to obtain the gauge transformation laws of the current densities $\mathbf{j}_p$ and $\mathbf{J}_{p\lambda}$. This will be presented in the next section.

3. The gauge transformation laws of the current densities

It should be noted that the gauge transformation laws given by equations (6.14) in [5] and also equations (6.4) in [8] are only valid for an infinitesimal local spin rotation [9]. In the following

we briefly describe how to generalize the result to a finite transformation. The paramagnetic current density $\mathbf{j}_p$ is calculated self-consistently from the N lowest one-particle eigenfunctions as follows (see equation (16)):

$$\mathbf{j}_p(\mathbf{r}) = \frac{\hbar}{2m\,\mathrm{i}} \sum_{j=1}^{N} \sum_{\sigma=\pm} [\psi_j^*(\mathbf{r},\sigma)\nabla\psi_j(\mathbf{r},\sigma) - \psi_j(\mathbf{r},\sigma)\nabla\psi_j^*(\mathbf{r},\sigma)] \tag{26}$$

where $\psi_j(\mathbf{r},\sigma)$ denotes a component of the two-spinor $|\psi_j\rangle$. Under a local $U(1)_{\mathrm{em}} \times SU(2)_{\mathrm{spin}}$ gauge transformation, $\psi_j(\mathbf{r},\sigma)$ transforms according to the law

$$\psi_j(\mathbf{r},\sigma) \to \psi_j'(\mathbf{r},\sigma) = \left[\exp\frac{\mathrm{i}e}{\hbar c}\Lambda_0(\mathbf{r})\right] \sum_{\sigma'=\pm} \langle\sigma|U_S|\sigma'\rangle\psi_j(\mathbf{r},\sigma'). \tag{27}$$

We recall that $U_S = \exp[(\mathrm{i}e/\hbar c)\Lambda(\mathbf{r})\cdot\boldsymbol{\sigma}]$. Now upon inverting equation (27) and inserting into equation (26), one thus obtains after some straightforward calculations the following result for the transformed paramagnetic current density:

$$\mathbf{j}_p \to \mathbf{j}_p' = \mathbf{j}_p + \frac{e}{mc} n\nabla\Lambda_0 - \mathrm{i}\frac{\hbar}{2m}\sum_{\mu=1}^{3} s_\mu \,\mathrm{Tr}_\sigma\left(\sigma_\mu U_S^{-1}\nabla U_S\right) \tag{28}$$

and for the paramagnetic spin current vector density

$$\mathbf{J}_{p\lambda} \to \mathbf{J}_{p\lambda}' = \sum_{\mu=1}^{3} R_{\lambda\mu}(\theta)\left[\mathbf{J}_{p\mu} + \frac{e}{mc} s_\mu \nabla\Lambda_0 - \mathrm{i}\frac{\hbar}{2m} n\,\mathrm{Tr}_\sigma\left(\sigma_\mu U_S^{-1}\nabla U_S\right)\right]. \tag{29}$$

It may easily be checked that for an infinitesimal $SU(2)_{\mathrm{spin}}$ transformation where the operator U_S can be written as $\left[I + \frac{\mathrm{i}}{2}\theta(\mathbf{u}\cdot\boldsymbol{\sigma})\right]$, the above general equations, (28) and (29), reduce to equations (6.14) of [5].

4. The equations of continuity

In the previous section we derived the transformation laws of the paramagnetic current densities $\mathbf{j}_p$ and $\mathbf{J}_{p\lambda}$ under the $U(1)_{\mathrm{em}} \times SU(2)_{\mathrm{spin}}$ gauge transformations. In [5] , it is shown that $\mathbf{j}_p$ satisfies an equation of continuity and $\mathbf{J}_{p\lambda}$ obeys a modified equation of continuity (see equations (6.8*a*) and (6.8*b*) of [5]). Since these equations were derived in the absence of the SOC vectors $\mathbf{A}_\lambda$, we propose therefore to generalize the result in the case where these vectors are present in the Hamiltonian. From the many-body Hamiltonian (5), we obtain the following exact equation for the paramagnetic current density $\mathbf{j}_p$:

$$\nabla\cdot\left[\mathbf{j}_p + \frac{e}{mc} n\mathbf{A} + \frac{e}{mc}\sum_{\lambda=1}^{3}\mathbf{A}_\lambda s_\lambda\right] = \mathbf{0} \tag{30}$$

and one obtains for the paramagnetic spin current density $\mathbf{J}_{p\lambda=1,2,3}$

$$\nabla\cdot\left[\mathbf{J}_{p\lambda} + \frac{e}{mc} s_\lambda\mathbf{A} + \frac{e}{mc} n\mathbf{A}_\lambda\right] = \frac{2}{\hbar}[\mathbf{V}\times\mathbf{s}]_\lambda + \frac{2e}{\hbar c}\sum_{\mu,\nu}\epsilon_{\lambda\mu\nu}\mathbf{A}_\mu\cdot\left[\mathbf{J}_{p\nu} + \frac{e}{mc}\mathbf{A}s_\nu\right] \tag{31}$$

where we recall that $\mathbf{V} = (e\hbar/2mc)\mathbf{B}$. As can be seen from the above equations, the vector $\mathbf{A}_\lambda$ enters in a linear manner. However, one notes the presence of additional SOC terms on the right-hand side of equation (31). Equations (30) and (31) are general and indeed reduce to those obtained by VR for vanishing SOC term.

As a final point related to the continuity equations, let us show that the various xc potentials $\mathbf{V}_{\mathrm{xc}}$, $\mathbf{A}_{\mathrm{xc}}$ and $\mathbf{A}_{\mathrm{xc}\lambda=1,2,3}$ defined respectively by equations (13)–(15) satisfy exact equations.

For that, using the one-electron equation (equation (16)), one can obtain a set of two equations of continuity satisfied by the current densities $\mathbf{j}_p$ and $\mathbf{J}_{p\lambda}$. These current densities are now calculated from the N lowest-lying one-electron wavefunctions

$$\nabla \cdot \left[\mathbf{j}_p + \frac{e}{mc}[\mathbf{A} + \mathbf{A}_{\rm xc}]n + \frac{e}{mc}\sum_{\lambda=1}^{3}[\mathbf{A}_\lambda + \mathbf{A}_{{\rm xc}\lambda}]s_\lambda \right] = \mathbf{0} \tag{32}$$

and

$$\nabla \cdot J_{p\lambda} + \frac{e}{mc}\nabla \cdot [(\mathbf{A} + \mathbf{A}_{\rm xc})s_\lambda + (\mathbf{A}_\lambda + \mathbf{A}_{{\rm xc}\lambda})n]$$
$$= \frac{2}{\hbar}[(\mathbf{V} + \mathbf{V}_{\rm xc}) \times \mathbf{s}]_\lambda + \frac{2e}{\hbar c}\sum_{\mu,\nu}\epsilon_{\lambda\mu\nu}\left[(\mathbf{A}_\mu + \mathbf{A}_{{\rm xc}\mu}) \cdot \mathbf{J}_{p\nu} + \frac{e}{mc}\mathbf{A} \cdot \mathbf{A}_\mu s_\nu\right]. \tag{33}$$

By requiring that the above two equations be compatible with equations (30) and (31), one obtains exact conditions on the xc potentials. These 'compatibility equations' are identical to those derived by VR (see equations (6.10*a*) and (6.10*b*) in [5]).

5. Summary

In this work, it has been explicitly shown how to include the spin–orbit coupling in the spin-current-density-functional theory. We have shown that the gauge transformations $U(1)_{\rm em} \times SU(2)_{\rm spin}$ are a symmetry of the problem. We have pointed out the necessity of including, in the formalism, the spin–orbit coupling in order to satisfy the full gauge invariance of the theory. The transformation laws of the currents under the finite local gauge transformations $U(1)_{\rm em} \times SU(2)_{\rm spin}$ have been given. These transformation laws reduce to those found for an infinitesimal transformation. Finally, the equations of continuity have been generalized to include the spin–orbit coupling.

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