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1989 J. Phys.: Condens. Matter 1 8445

(http://iopscience.iop.org/0953-8984/1/44/015)

J. Phys.: Condens. Matter 1 (1989) 8445–8451. Printed in the UK

Relativistic Kohn–Sham formalism and the microscopic stress tensor

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Received 3 October 1988, in final form 19 June 1989

Abstract. After a short review of the Kohn–Sham procedure for a system of relativistic charged particles a relativistic extension of the local density approximation is presented. In contrast to former proposals, it satisfies the requirement of Lorentz invariance. Within this relativistic Kohn–Sham theory the microscopic stress tensor is considered and the corresponding complete energy–momentum tensor is constructed. A local expression is found in accordance with the assumptions about the energy density.

1. Introduction

The ground state of a system of non-relativistic interacting particles in an arbitrary external potential obeys the Hohenberg–Kohn theorem (Hohenberg and Kohn 1964) according to which all ground-state quantities and in particular the energy are unique functionals of the particle density n. Kohn and Sham (1965) invented a procedure to associate effective one-particle states with the ground state of the interacting system. A relativistic generalisation of the Hohenberg–Kohn theorem has been given by Rajagopal and Callaway (1973). In this case the external potential must be replaced by an external 4-potential (or corresponding electric and magnetic fields) and instead of density functionals one has functionals of the 4-current density. The corresponding Kohn–Sham scheme has been formulated by Rajagopal (1978) and by Eschrig *et al* (1985). The latter authors also proposed a relativistic version of the local density approximation by introducing an additional dependence on the magnetisation vector (instead of the current density) in the XC energy. A disadvantage of their *ansatz*, however, is the lack of Lorentz invariance. Therefore in § 3 of this paper we present a modified version of the relativistic local approximation ensuring Lorentz invariance.

Nielsen and Martin (1985) and recently Ziesche *et al* (1988a, b) investigated the microscopic stress tensor within the framework of the non-relativistic local density approximation and constructed an XC part of the stress tensor which turned out to be also a function of the local density. Sections 4 and 5 of this work are devoted to a relativistic generalisation of the XC stress tensor based on the local approximation introduced in § 3. The resulting stress tensor is again a local expression, which can be complemented to an energy–momentum tensor showing the correct covariant behaviour under Lorentz transformation.

0953-8984/89/448445 + 07 $02.50

2. Relativistic Kohn–Sham formalism

We start with a short review of the relativistic version of the Kohn–Sham formalism previously outlined in Eschrig *et al* (1985). We consider a system of charged particles with electromagnetic interaction in an external field described by a 4-potential

$$A^{\mu}_{\text{ext}}(\boldsymbol{r}) = (\Phi_{\text{ext}}/c, \boldsymbol{A}_{\text{ext}}). \tag{2.1}$$

According to the relativistic Hohenberg–Kohn theorem (Rajagopal and Callaway 1973) the ground-state energy is a unique functional of the current density

$$j^{\mu}(\boldsymbol{r}) = (\rho c, \boldsymbol{j}) \qquad j_{\mu}(\boldsymbol{r}) = (\rho c, -\boldsymbol{j}) \tag{2.2}$$

where ρ denotes the charge density and $\boldsymbol{j}$ is the total current density comprising both the orbital and spin contributions. In the sense of the Kohn–Sham procedure the ground-state energy may be split up into

$$E = T + E_{\text{H}} + E_{\text{XC}} + \int \mathrm{d}^3 r \rho \Phi_{\text{ext}} \tag{2.3}$$

where T is the kinetic (and rest) energy of effective one-particle states

$$T = \sum_k \left\langle \varphi_k \middle| \boldsymbol{\alpha} c \left(\frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial \boldsymbol{r}} + |e| \boldsymbol{A} \right) + mc^2 \beta \middle| \varphi_k \right\rangle. \tag{2.4}$$

The φ_k are chosen in such a way that they yield the correct current density

$$j^{\mu} = -|e| c \sum_k \bar{\varphi}_k \gamma^{\mu} \varphi_k. \tag{2.5}$$

The mean field $\boldsymbol{A} = \boldsymbol{A}_{\text{ext}} + \boldsymbol{A}_{\text{H}}$ consists of the external and the Hartree fields. The latter is the expectation value of the field produced by the particles themselves and its sources are given by j^{μ}. The term E_{H} in (2.3) represents the energy of this Hartree field

$$E_{\text{H}} = \tfrac{1}{2} \int \mathrm{d}^3 r \left(\varepsilon_0 \boldsymbol{E}^2_{\text{H}} + \frac{1}{\mu_0} \boldsymbol{B}^2_{\text{H}} \right) = \tfrac{1}{2} \int \mathrm{d}^3 r [\rho \Phi_{\text{H}} + \boldsymbol{j} \boldsymbol{A}_{\text{H}}]. \tag{2.6}$$

The quantity E_{XC} comprises all correlation and exchange effects. The last term in (2.3) is the energy in the external field. Expression (2.3) may be transformed into

$$\begin{aligned} E &= T_0 + E_{\text{XC}} + \int \mathrm{d}^3 r j_{\mu} (\tfrac{1}{2} A^{\mu}_{\text{H}} + A^{\mu}_{\text{ext}}) \\ T_0 &= \sum_k \left\langle \varphi_k \middle| \boldsymbol{\alpha} c \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial \boldsymbol{r}} + mc^2 \beta \middle| \varphi_k \right\rangle. \end{aligned} \tag{2.7}$$

A variation with respect to the one-particle states and, consequently, to the current density j^{μ} yields

$$\delta E = \delta T_0 + \delta E_{\text{XC}} + \int \mathrm{d}^3 r \delta j_{\mu} (A^{\mu}_{\text{H}} + A^{\mu}_{\text{ext}}). \tag{2.8}$$

Defining the XC potentials by

$$\begin{aligned} \delta E_{\text{XC}}[j^{\mu}] &= \int \mathrm{d}^3 r \delta j_{\mu}(\boldsymbol{r}) \frac{\delta E_{\text{XC}}}{\delta j_{\mu}(\boldsymbol{r})} = \int \mathrm{d}^3 r \delta j_{\mu} A^{\mu}_{\text{XC}} \\ A^{\mu}_{\text{XC}}(\boldsymbol{r}) &= \frac{\delta E_{\text{XC}}}{\delta j_{\mu}(\boldsymbol{r})} \qquad \Phi_{\text{XC}} = \frac{\delta E_{\text{XC}}}{\delta \rho} \qquad \boldsymbol{A}_{\text{XC}} = -\frac{\delta E_{\text{XC}}}{\delta \boldsymbol{j}} \end{aligned} \tag{2.9}$$

we obtain the following equations for the Kohn–Sham states:

$$\left[\boldsymbol{\alpha}c\left(\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial \boldsymbol{r}}+|e|\boldsymbol{A}+|e|\boldsymbol{A}_{\mathrm{XC}}\right)-|e|\Phi-|e|\Phi_{\mathrm{XC}}+mc^2\beta\right]\varphi_k=\varepsilon_k\varphi_k. \tag{2.10}$$

Let us note that the paper by Eschrig *et al* (1985) contains an erroneous sign in the definitions of $\boldsymbol{A}_{\mathrm{XC}}$ and $\boldsymbol{B}_{\mathrm{XC}}$.

3. Local approximation

Generalising the usual local density approximation, Eschrig *et al* (1985) proposed the following *ansatz* for the correlation-exchange energy:

$$E_{\mathrm{XC}}[j^\mu]=\int \mathrm{d}^3r n\varepsilon_{\mathrm{XC}}(n,|\boldsymbol{M}|) \tag{3.1}$$

where n and $\boldsymbol{M}$ denote the particle density and the magnetisation vector, respectively. Analogously to $\boldsymbol{j}$ the magnetisation $\boldsymbol{M}$ contains spin as well as orbital contributions. An unsatisfactory feature of assumption (3.1) is the lack of Lorentz invariance. In fact, n and $\boldsymbol{M}$ are components of 4-quantities. Therefore, expression (3.1) for the energy density can be valid only in a special reference system, probably in the local rest frame ($\boldsymbol{j}=0$). In order to overcome this problem, we write instead of (3.1)

$$E_{\mathrm{XC}}=\int \mathrm{d}^3r e_{\mathrm{XC}}(j^\mu,M^{\mu\nu})=\int \mathrm{d}^3r e_{\mathrm{XC}}(\rho,\boldsymbol{j},\boldsymbol{P},\boldsymbol{M}). \tag{3.2}$$

The 4-tensor $M^{\mu\nu}$ consists of the components

$$M^{\mu\nu}=\left(\begin{array}{c|ccc} 0 & -P_1c & -P_2c & -P_3c \\ \hline P_1c & 0 & M_3 & -M_2 \\ P_2c & -M_3 & 0 & M_1 \\ P_3c & M_2 & -M_1 & 0 \end{array}\right) \tag{3.3}$$

and is connected with the current density by the relations

$$j^\mu=\partial_\nu M^{\mu\nu} \qquad \rho=-\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{r}} \qquad \boldsymbol{j}=\frac{\partial}{\partial \boldsymbol{r}}\times\boldsymbol{M}+\dot{\boldsymbol{P}}. \tag{3.4}$$

The time derivative of the polarisation vector $\boldsymbol{P}$ vanishes for the time-independent ground state.

A variation of E_{XC} now leads to

$$\begin{aligned}\delta E_{\mathrm{XC}}&=\int \mathrm{d}^3r\left(\delta\rho\frac{\partial e_{\mathrm{XC}}}{\partial\rho}+\delta\boldsymbol{j}\frac{\partial e_{\mathrm{XC}}}{\partial\boldsymbol{j}}+\delta\boldsymbol{M}\frac{\partial e_{\mathrm{XC}}}{\partial\boldsymbol{M}}+\delta\boldsymbol{P}\frac{\partial e_{\mathrm{XC}}}{\partial\boldsymbol{P}}\right)\\&=\int \mathrm{d}^3r\left[\delta\boldsymbol{P}\left(\frac{\partial}{\partial\boldsymbol{r}}\frac{\partial e_{\mathrm{XC}}}{\partial\rho}+\frac{\partial e_{\mathrm{XC}}}{\partial\boldsymbol{P}}\right)+\delta\boldsymbol{M}\left(\frac{\partial}{\partial\boldsymbol{r}}\times\frac{\partial e_{\mathrm{XC}}}{\partial\boldsymbol{j}}+\frac{\partial e_{\mathrm{XC}}}{\partial\boldsymbol{M}}\right)\right].\end{aligned} \tag{3.5}$$

In the last line the variations of ρ and $\boldsymbol{j}$ are expressed by the aid of (3.4) and an integration by parts is carried out. Alternatively we have according to (2.9)

$$\begin{aligned}\delta E_{\mathrm{XC}}&=\int \mathrm{d}^3r\delta j_\mu A^\mu_{\mathrm{XC}}=\int \mathrm{d}^3r\,\partial^\nu\delta M_{\mu\nu}A^\mu_{\mathrm{XC}}\\&=-\int \mathrm{d}^3r\tfrac{1}{2}\delta M_{\mu\nu}F^{\mu\nu}_{\mathrm{XC}}=-\int \mathrm{d}^3r(\delta\boldsymbol{P}\boldsymbol{E}_{\mathrm{XC}}+\delta\boldsymbol{M}\boldsymbol{B}_{\mathrm{XC}})\end{aligned} \tag{3.6}$$

where the field tensor

$$F^{\mu\nu}_{\mathrm{XC}} = \partial^{\nu} A^{\mu}_{\mathrm{XC}} - \partial^{\mu} A^{\nu}_{\mathrm{XC}} \qquad F^{\mu\nu}_{\mathrm{XC}} = \left(\begin{array}{c|ccc} 0 & E^1_{\mathrm{XC}}/c & E^2_{\mathrm{XC}}/c & E^3_{\mathrm{XC}}/c \\ \hline -E^1_{\mathrm{XC}}/c & 0 & B^3_{\mathrm{XC}} & -B^2_{\mathrm{XC}} \\ -E^2_{\mathrm{XC}}/c & -B^3_{\mathrm{XC}} & 0 & B^1_{\mathrm{XC}} \\ -E^3_{\mathrm{XC}}/c & B^2_{\mathrm{XC}} & -B^1_{\mathrm{XC}} & 0 \end{array}\right)$$

$$\boldsymbol{B}_{\mathrm{XC}} = \frac{\partial}{\partial \boldsymbol{r}} \times \boldsymbol{A}_{\mathrm{XC}} \qquad \boldsymbol{E}_{\mathrm{XC}} = -\frac{\partial \Phi_{\mathrm{XC}}}{\partial \boldsymbol{r}} - \dot{\boldsymbol{A}}_{\mathrm{XC}} = -\frac{\partial \Phi_{\mathrm{XC}}}{\partial \boldsymbol{r}} \tag{3.7}$$

has been introduced. A comparison between (3.5) and (3.6) yields

$$\boldsymbol{E}_{\mathrm{XC}} = -\frac{\partial e_{\mathrm{XC}}}{\partial \boldsymbol{P}} - \frac{\partial}{\partial \boldsymbol{r}} \frac{\partial e_{\mathrm{XC}}}{\partial \rho} \qquad \boldsymbol{B}_{\mathrm{XC}} = -\frac{\partial e_{\mathrm{XC}}}{\partial \boldsymbol{M}} - \frac{\partial}{\partial \boldsymbol{r}} \times \frac{\partial e_{\mathrm{XC}}}{\partial \boldsymbol{j}} \tag{3.8}$$

$$F^{\mu\nu}_{\mathrm{XC}} = \frac{\partial e_{\mathrm{XC}}}{\partial M_{\nu\mu}} + \frac{\partial}{\partial x_{\nu}} \frac{\partial e_{\mathrm{XC}}}{\partial j_{\mu}} - (\nu \leftrightarrow \mu).$$

Owing to the definition (3.7), the XC fields have to satisfy the following equations:

$$\frac{\partial \boldsymbol{B}_{\mathrm{XC}}}{\partial \boldsymbol{r}} = -\frac{\partial}{\partial \boldsymbol{r}} \frac{\partial e_{\mathrm{XC}}}{\partial \boldsymbol{M}} = 0 \qquad \frac{\partial}{\partial \boldsymbol{r}} \times \boldsymbol{E}_{\mathrm{XC}} = -\frac{\partial}{\partial \boldsymbol{r}} \times \frac{\partial e_{\mathrm{XC}}}{\partial \boldsymbol{P}} = 0. \tag{3.9}$$

These conditions together with (3.4) completely determine the polarisation $\boldsymbol{P}$ and magnetisation $\boldsymbol{M}$ for a given set of Kohn–Sham states φ_k with corresponding ρ and $\boldsymbol{j}$. There is no possibility of imposing an additional gauge condition on $\boldsymbol{M}$ as was done by Eschrig *et al* (1985).

From (3.8) one can see that e_{XC} has to be a 4-scalar. That means it can only depend on invariants constructed from the 4-quantities j^{μ} and $M^{\mu\nu}$. In analogy with (3.1) we shall restrict ourselves to two invariants describing the charge density ρ_0 and magnetisation M_0 in the local rest frame ($j = 0$). To this end we consider the 4-vectors j^{μ} and

$$g_{\mu} := \frac{1}{2c} \varepsilon_{\mu\nu\kappa\lambda} j^{\nu} M^{\kappa\lambda} = \left(\frac{\boldsymbol{jM}}{c}, -\boldsymbol{g}\right)$$
$$\boldsymbol{g} = \boldsymbol{j} \times \boldsymbol{P} + \rho \boldsymbol{M} \tag{3.10}$$

where $\varepsilon_{\mu\nu\kappa\lambda}$ is the completely antisymmetric Levi-Civita tensor, and square them:

$$\zeta = \frac{1}{2c^2} j^{\mu} j_{\mu} = \tfrac{1}{2}(\rho^2 - \boldsymbol{j}^2/c^2) = \tfrac{1}{2}\rho_0^2$$
$$\eta = -\tfrac{1}{2} g^{\mu} g_{\mu} = \tfrac{1}{2}[(\boldsymbol{j} \times \boldsymbol{P} + \rho \boldsymbol{M})^2 - (\boldsymbol{jM}/c)^2] = \tfrac{1}{2}\rho_0^2 M_0^2. \tag{3.11}$$

Now, the energy density e_{XC} is assumed to depend only on these invariant quantities

$$e_{\mathrm{XC}} = e_{\mathrm{XC}}(\zeta, \eta). \tag{3.12}$$

In order to calculate the XC fields, we need the derivatives

$$\frac{\partial \zeta}{\partial \rho} = \rho \qquad \frac{\partial \zeta}{\partial \boldsymbol{j}} = -\frac{1}{c^2} \boldsymbol{j}$$

$$\frac{\partial \eta}{\partial \rho} = \boldsymbol{Mg} \qquad \frac{\partial \eta}{\partial \boldsymbol{j}} = \boldsymbol{p} \times \boldsymbol{g} - \frac{1}{c^2} \boldsymbol{M}(\boldsymbol{jM})$$

$$\frac{\partial \eta}{\partial \boldsymbol{P}} = \boldsymbol{g} \times \boldsymbol{j} \qquad \frac{\partial \eta}{\partial \boldsymbol{M}} = \rho \boldsymbol{g} - \frac{1}{c^2} \boldsymbol{j}(\boldsymbol{jM}).$$

The difference from the XC fields proposed by Eschrig *et al* (1985) is twofold. First the density ρ and magnetisation M in e_{XC} are replaced by Lorentz-invariant quantities ρ_0

and M_0 and, secondly, additional terms containing derivatives with respect to $\boldsymbol{P}$ and $\boldsymbol{j}$ occur in (3.8). The contributions of $\boldsymbol{P}$ in (3.10) and (3.11) could possibly be of the same order of magnitude as those of $\boldsymbol{M}$.

4. Microscopic stress tensor

In recent papers Ziesche *et al* (1988a, b) considered the microscopic stress tensor within the non-relativistic local density approximation and found an XC part

$$\sigma_{XC} = -n^2 \frac{\mathrm{d}\varepsilon_{\mathrm{XC}}}{\mathrm{d}n} I \tag{4.1}$$

where $\varepsilon_{\mathrm{XC}}$ is the XC energy per particle and I denotes the unit tensor. To treat the relativistic case we put

$$\begin{aligned}
\sigma &= \sigma_{\mathrm{KS}} + \sigma_{\mathrm{H}} + \sigma_{\mathrm{XC}} \\
\sigma_{\mathrm{KS}} &= -\sum_k \varphi_k^{\dagger}(\boldsymbol{r}) c\boldsymbol{\alpha} \otimes \left[\frac{\hbar}{2\mathrm{i}}\left(\frac{\overrightarrow{\partial}}{\partial \boldsymbol{r}} - \frac{\overleftarrow{\partial}}{\partial \boldsymbol{r}}\right) + |e|\boldsymbol{A}\right]\varphi_k(\boldsymbol{r}) \\
\sigma_{\mathrm{H}} &= \varepsilon_0 \boldsymbol{E}_{\mathrm{H}} \otimes \boldsymbol{E}_{\mathrm{H}} + \frac{1}{\mu_0}\boldsymbol{B}_{\mathrm{H}} \otimes \boldsymbol{B}_{\mathrm{H}} - \tfrac{1}{2} I\left(\varepsilon_0 \boldsymbol{E}_{\mathrm{H}}^2 + \frac{1}{\mu_0}\boldsymbol{B}_{\mathrm{H}}^2\right).
\end{aligned} \tag{4.2}$$

Here, σ_{KS} represents the (negative) momentum-flux tensor of the Kohn–Sham states. The arrows above the nabla operators indicate the functions on which they act. The second part σ_{H} is the Maxwell stress tensor of the Hartree field. The XC part σ_{XC} is unknown. The total stress tensor has to obey the equilibrium condition

$$\frac{\partial \sigma}{\partial \boldsymbol{r}} = -\boldsymbol{f}_{\mathrm{ext}} = -(\rho \boldsymbol{E}_{\mathrm{ext}} + \boldsymbol{j} \times \boldsymbol{B}_{\mathrm{ext}}). \tag{4.3}$$

The divergences of σ_{KS} and σ_{H} can be calculated from the expressions (4.2) by using the Kohn–Sham and Maxwell equations

$$\frac{\partial \sigma_{\mathrm{KS}}}{\partial \boldsymbol{r}} = -\boldsymbol{f}_{\mathrm{H}} - \boldsymbol{f}_{\mathrm{ext}} - \boldsymbol{f}_{\mathrm{XC}} - \frac{\partial}{\partial \boldsymbol{r}}(\boldsymbol{j} \otimes \boldsymbol{A}_{\mathrm{XC}}) \qquad \frac{\partial \sigma_{\mathrm{H}}}{\partial \boldsymbol{r}} = \boldsymbol{f}_{\mathrm{H}} \tag{4.4}$$

where $\boldsymbol{f}_{\mathrm{H}}$ and $\boldsymbol{f}_{\mathrm{XC}}$ are defined analogously to (4.3) with the Hartree and XC fields, respectively. For σ_{XC} follows

$$\frac{\partial \sigma_{\mathrm{XC}}}{\partial \boldsymbol{r}} = \boldsymbol{f}_{\mathrm{XC}} + \frac{\partial}{\partial \boldsymbol{r}}(\boldsymbol{j} \otimes \boldsymbol{A}_{\mathrm{XC}}). \tag{4.5}$$

Taking into account the definitions (3.7) of $\boldsymbol{B}_{\mathrm{XC}}$, $\boldsymbol{E}_{\mathrm{XC}}$, the relations (3.4) between j^{μ} and $M^{\mu\nu}$ and the continuity equation $\mathrm{div}\,\boldsymbol{j} = 0$, we may transform the right-hand side of (4.5) into a divergence and identify the resulting tensor with the stress tensor σ_{XC}. This leads to

$$\begin{aligned}
\sigma_{\mathrm{XC}} = \boldsymbol{j} \otimes \boldsymbol{A}_{\mathrm{XC}} &+ I\left(e_{\mathrm{XC}} - \rho\frac{\partial e_{\mathrm{XC}}}{\partial \rho} - \boldsymbol{j}\frac{\partial e_{\mathrm{XC}}}{\partial \boldsymbol{j}} - \boldsymbol{P}\frac{\partial e_{\mathrm{XC}}}{\partial \boldsymbol{P}}\right) + \boldsymbol{j} \otimes \frac{\partial e_{\mathrm{XC}}}{\partial \boldsymbol{j}} \\
&+ \boldsymbol{P} \otimes \frac{\partial e_{\mathrm{XC}}}{\partial \boldsymbol{P}} - \frac{\partial e_{\mathrm{XC}}}{\partial \boldsymbol{M}} \otimes \boldsymbol{M}.
\end{aligned} \tag{4.6}$$

Insertion of the special assumption (3.12) for the XC energy gives

$$\sigma_{\mathrm{XC}} = \boldsymbol{j} \otimes \boldsymbol{A}_{\mathrm{XC}} + I e_{\mathrm{XC}} - \frac{\partial e_{\mathrm{XC}}}{\partial \zeta}\left[2\zeta I + \frac{1}{c^2}\boldsymbol{j} \otimes \boldsymbol{j}\right] - \frac{\partial e_{\mathrm{XC}}}{\partial \rho}[2\rho I + \boldsymbol{g} \otimes \boldsymbol{g}]. \tag{4.7}$$

Let us emphasise that in accordance with our local approximation for the energy density e_{XC} we also find local expressions (4.6) and (4.7) for the corresponding stress tensor.

5. Energy–momentum tensor

In a relativistic formulation the stress tensor has to be the spatial part of the energy–momentum tensor $T^{\mu\nu}$

$$T^{kl} = -\sigma^{kl} \qquad k, l = 1, 2, 3. \tag{5.1}$$

We may split up the tensor $T^{\mu\nu}$ in the same way as we did for σ in (4.2):

$$T^{\mu\nu} = T^{\mu\nu}_{KS} + T^{\mu\nu}_{H} + T^{\mu\nu}_{XC}. \tag{5.2}$$

The four-dimensional generalisations of the stress tensors (4.2) and (4.6) are straightforward and lead to

$$\begin{aligned}
T^{\mu\nu}_{KS} &= -\frac{c\hbar}{2\mathrm{i}}(\partial^{\nu} - \partial'^{\nu}) \sum_k \bar{\varphi}_k(x')\gamma^{\mu}\varphi_k(x)\Big|_{x=x'} + |e|cA^{\nu} \sum_k \bar{\varphi}_k\gamma^{\mu}\varphi_k \\
T^{\mu\nu}_{H} &= \frac{1}{\mu_0}[F^{\mu\kappa}_{H} F_{H\kappa}{}^{\nu} + \tfrac{1}{4}g^{\mu\nu} F_H{}^{\kappa\lambda} F_{H\kappa\lambda}] \\
T^{\mu\nu}_{XC} &= -j^{\mu} A^{\mu}_{XC} + g^{\mu\nu}\left(e_{XC} - j^{\kappa}\frac{\partial e_{XC}}{\partial j^{\kappa}} - M^{\kappa\lambda}\frac{\partial e_{XC}}{\partial M^{\kappa\lambda}}\right) \\
&\quad + j^{\mu}\frac{\partial e_{XC}}{\partial j_{\nu}} - M^{\mu\kappa}\frac{\partial e_{XC}}{\partial M^{\kappa}{}_{\nu}} - M^{\kappa\mu}\frac{\partial e_{XC}}{\partial M_{\nu}{}^{\kappa}}.
\end{aligned} \tag{5.3}$$

The metric tensor $g^{\mu\nu}$ is defined by

$$g^{00} = -g^{11} = -g^{22} = -g^{33} = 1 \qquad g_{ik} = 0 \qquad (i \neq k).$$

With the special choice (3.12) $T^{\mu\nu}_{XC}$ becomes

$$T^{\mu\nu}_{XC} = -j^{\mu}A^{\nu}_{XC} + g^{\mu\nu}e_{XC} - \frac{\partial e_{XC}}{\partial \zeta}[2\zeta g^{\mu\nu} - j^{\mu}j^{\nu}/c^2] - \frac{\partial e_{XC}}{\partial \rho}[2\rho g^{\mu\nu} - g^{\mu}g^{\nu}]. \tag{5.4}$$

The total energy–momentum tensor satisfies the balance equation

$$\partial_{\mu} T^{\mu\nu} = f^{\nu}_{ext} = (\boldsymbol{j}\boldsymbol{E}_{ext}/c, \boldsymbol{f}_{ext}). \tag{5.5}$$

We may check the correctness of our construction by examining the component T^{00} of the energy–momentum tensor. This component must represent the energy density. After some transformations we find for the XC part of (5.3)

$$T^{00}_{XC} = e_{XC} - \rho\Phi_{XC} + \boldsymbol{j}\boldsymbol{A}_{XC} - \frac{\partial}{\partial \boldsymbol{r}}\left[\boldsymbol{M} \times \left(\boldsymbol{A}_{XC} + \frac{\partial e_{XC}}{\partial \boldsymbol{j}}\right)\right]. \tag{5.6}$$

The last term is a divergence and, therefore, does not contribute to the energy. The total energy may be obtained from (5.3) and (5.6) by using the Kohn–Sham equation (2.10)

$$\int \mathrm{d}^3 r T^{00} = T + E_H + E_{XC}. \tag{5.7}$$

A comparison with (2.3) shows that this is indeed the energy of the ground state assumed at the beginning, but without the energy in the external field. This energy, however,

may also be included by transforming the right-hand side of (5.5) and subtracting it from the left-hand side

$$\boldsymbol{j}\boldsymbol{E}_{\text{ext}} = -\boldsymbol{j}\frac{\partial}{\partial \boldsymbol{r}}\Phi_{\text{ext}} = -\frac{\partial}{\partial \boldsymbol{r}}(\boldsymbol{j}\Phi_{\text{ext}}) + \frac{\partial \boldsymbol{j}}{\partial \boldsymbol{r}}\Phi_{\text{ext}}$$

$$= -\frac{\partial}{\partial \boldsymbol{r}}(\boldsymbol{j}\Phi_{\text{ext}}) - \frac{\partial \rho}{\partial t}\Phi_{\text{ext}} = -\partial_\mu(j^\mu \Phi_{\text{ext}}) \tag{5.8}$$

$\partial_\mu(T^{\mu 0} + j^\mu \Phi_{\text{ext}}/c) = 0.$

Thus we find an energy density $T^{00} + \rho\Phi_{\text{ext}}$ in complete agreement with (2.3).

6. Conclusion

In this paper we extended the local density approximation to the relativistic case in such a way that Lorentz invariance is ensured. Moreover we constructed the corresponding stress and energy–momentum tensors. The question of whether the local approximation for a system of relativistic electrons is reasonable or not remains open. Also we disregarded the problem of how to choose the XC part of the energy density. In general it can be a function of all invariant combinations of the 4-quantities j^μ and $M^{\mu\nu}$. It seems necessary to take into account at least two of these invariants characterising the charge density and magnetisation in the local rest frame. In doing so, we may use expressions derived in the literature for the XC energy of spin-polarised systems (MacDonald 1983, Bu Xing Xu *et al* 1984) where the particle density and the spin density have to be replaced by the corresponding invariant quantities ρ_0 and M_0 defined in (3.11).

Acknowledgment

The authors are indebted to Professor P Ziesche for suggesting the present work and for his encouraging interest.

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