On the path-dependent polarisation tensor

1985 J. Phys. A: Math. Gen. 18 437

(http://iopscience.iop.org/0305-4470/18/3/019)

J. Phys. A: Math. Gen. **18** (1985) 437-443. Printed in Great Britain

On the path-dependent polarisation tensor

Marek Żukowski
Instytut Fizyki Teoretycznej i Astrofizyki, Uniwersytet Gdański, Wita Stwosza 57, 80-952 Gdańsk, Poland

Received 16 February 1981, in final form 6 August 1984

Abstract. A generalised definition of the path-dependent polarisation tensor is given. The definition is applicable for various descriptions of charged particles constituting a neutral atom.

1. Introduction

When neutral atoms and molecules are considerd it is often very convenient to introduce a polarisation tensor $m^{\alpha\beta}$ in place of the current density four-vector j^{α}. Although the notion of the polarisation tensor has previously been used only in macroscopic electrodynamics, it can also be very useful in the electrodynamics of atoms and molecules. In this theory atoms and molecules are usually described as non-relativistic objects, and since the Coulomb field is an excellent approximation to the interaction of slowly moving charges, the Coulomb gauge formalism is employed for the description of the field. However, the multipolar interaction Hamiltonian has always been an interesting alternative, mainly due to its manifestly gauge-independent form (Power and Zienau 1957, 1959).

In the multipolar formalism the interaction term of the Lagrangian is given by

$$\frac{1}{2}\int m^{\alpha\beta} f_{\alpha\beta}\, \mathrm{d}^3x \tag{1}$$

where $f_{\alpha\beta}$ is the tensor of the electromagnetic field. The problem of representing microscopic charge and current densities for point particles in terms of polarisation tensors has been solved by de Groot and his co-workers (de Groot and Stuttorp 1972, de Groot 1969) in their study of the modern version of the Lorentz programme, i.e. the derivation of the macroscopic laws of electromagnetism from microscopic electrodynamics. Their tensor $m^{\alpha\beta}$ has been given in the form of a multipole expansion. However, it has been shown (Power and Thirunamachandran 1971, Babiker *et al* 1973, 1974, Babiker 1975, Woolley 1971, 1975a, b, Healy 1977) that one can obtain exact expressions for the magnetisation and polarisation vectors $\boldsymbol{m}$ and $\boldsymbol{p}$. These have the so-called path-dependent form.

This path-dependent representation for the polarisation and magnetisation vectors can be written in a manifestly co-variant form (Fiutak and Żukowski 1978, Healy 1978). For the simplest case of the hydrogen atom, the polarisation tensor is given by

$$m^{\alpha\beta}(x) = e\int_{\Sigma} \delta^{(4)}(x-\xi)\, \mathrm{d}\sigma^{\alpha\beta} \tag{2}$$

0305-4470/85/030437+07\$02.25

where e is the charge of the electron, and Σ is an arbitrary surface spanned between the trajectories of the nucleus and the electron.

However, formula (2) can be used only for electrodynamics of point particles. We shall present here a generalisation of the path-dependent tensor, which can be applied to a very wide class of descriptions of charges, ranging from point particles to second quantised charged fields. The formulae will be given for a single neutral atom.

2. The polarisation tensor

The polarisation tensor is defined as an antisymmetric solution of the equation

$$\partial_\beta m^{\alpha\beta} = j^\alpha, \tag{3}$$

where the current obeys the continuity equation

$$\partial_\alpha j^\alpha = 0. \tag{4}$$

We shall assume here that the total charge carried by j^μ is zero, i.e.

$$\int_\sigma \mathrm{d}\sigma^\mu j_\mu = 0 = Q, \tag{5}$$

where σ is an arbitrary space-like hypersurface. No other assumptions on the properties of j^μ will be made here. The particular form j^μ is completely arbitrary.

Let us consider the kernel F defined by

$$F^{\alpha\beta}_\rho(z|x) = \int_{R(x)}^x \mathrm{d}\xi^{[\alpha}\delta^{(4)}(z-\xi)\,\partial\xi^{\beta]}/\partial x^\alpha. \tag{6}$$

The path of integration in (6), $\xi(x)$, is space-like. It begins at the point $R(x)$, and ends at x. $R(x)$ plays the role of a privileged 'central' point. We assume that there exists a privileged reference frame in which $R(x)$ fulfils the following conditions:

$$\partial R^\mu(x)/\partial x^0 = n^\mu, \qquad \partial R^\mu(x)/\partial x^i = 0 \qquad (i=1,2,3), \qquad R^0 = x^0, \tag{7}$$

where n^μ is a unit time-like vector which defines the reference frame. In this frame of reference $\xi(x)$ is a path with a constant time coordinate, i.e. $\xi^0(x) = x^0$. However, as we shall see below, this condition may be relaxed for a certain class of solutions.

We shall prove that

$$m^{\alpha\beta}(z) = \int_{\sigma_1}^{\sigma_2} F^{\alpha\beta}_\rho(z|x) j^\rho(x)\,\mathrm{d}^4x \tag{8}$$

is a solution of the equation (3), for all z belonging to a region Ω of the spacetime between two space-like hypersurfaces σ_1 and σ_2. These hypersurfaces are hyperplanes with their normal four-vectors parallel to n^μ. We assume σ_2 to be later than σ_1. In order to get a solution of (3) for the whole spacetime one should consider σ_1 and σ_2 to be situated at the temporal minus and plus infinity, respectively. Such a procedure can be denoted as $\sigma_1 \to \sigma(-\infty)$ and $\sigma_2 \to \sigma(+\infty)$.

The antisymmetry of (8) stems from the very definition of F.

It is convenient to parametrise the path joining $R(x)$ with x:

$$F^{\alpha\beta}_\rho(z|x) = \int_0^1 \mathrm{d}l\,\mathrm{d}\xi^{[\alpha}(x,l)/\mathrm{d}l\,\delta^{(4)}(z-\xi(x,l))\,\partial\xi^{\beta]}(x,l)/\partial x^\rho \tag{9}$$

where $\xi(x,1)=x$ and $\xi(x,0)=R(x)$. We now note that

$$\partial_\beta \int_{\sigma_1}^{\sigma_2} F_\rho^{\alpha\beta}(z|x) j^\rho(x)\,\mathrm{d}^4x$$
$$= \int_{\sigma_1}^{\sigma_2} \mathrm{d}^4x \int_0^1 [(\mathrm{d}/\mathrm{d}l)\delta^{(4)}(z-\xi(x,l))\,\partial\xi^\alpha(x,l)/\partial x^\rho j^\rho(x)]\,\mathrm{d}l$$
$$- \int_{\sigma_1}^{\sigma_2} \mathrm{d}^4x \int_0^1 \mathrm{d}l\,\mathrm{d}\xi^\alpha(x,l)/\mathrm{d}l\,\partial/\partial x^\rho\,\delta^{(4)}(z-\xi) j^\rho(x). \qquad (10)$$

One can integrate both expressions by parts; the first one over l, and the second one over x. It is convenient to transform the result to the privileged reference frame. This leads to

$$\int_{\sigma_1}^{\sigma_2} \mathrm{d}^4x[\delta^{(4)}(z-x)\delta_\rho^\beta j^\rho(x) - \delta^{(4)}(z-(R(x))\delta_0^\beta j^0(x)]$$
$$= j^\beta(z) - \int_{x_1^0}^{x_2^0} \mathrm{d}x^0\,\delta(z^0-x^0)\int_{\sigma(x^0)} \mathrm{d}\sigma_0\, j^0(x)\delta^{(3)}(z-\boldsymbol{R})\delta_0^\beta$$
$$= j^\beta(z) - \delta_0^\beta\delta^{(3)}(z-R)Q = j^\beta(z). \qquad (11)$$

From (11) one can see that (8) is a solution of (3). The surface term, which results when one integrates the second term of (10) by parts, vanishes, since z belongs to the interior of the region Ω, and the integration paths are inside the hypersurfaces $\sigma_1=\sigma(x_1^0)$ and $\sigma_2=\sigma(x_2^0)$.

A general solution of (3) inside Ω is the sum of (8) and the general solution of the homogeneous equation

$$\partial_\beta\psi^{\alpha\beta}=0 \qquad (12)$$

with the condition that $\psi^{\alpha\beta}=-\psi^{\beta\alpha}$. Indeed, each $m^{\alpha\beta}$ of such a form obviously satisfies (3), and conversely, each solution of (3) may be written in this form. To prove that statement, let us multiply equation (3) by F and integrate with respect to x over the region Ω:

$$\int_{\sigma_1}^{\sigma_2} F_\beta^{\mu\nu}(z|x)\partial_\alpha m^{\beta\alpha}(x)\,\mathrm{d}^4x = \int_{\sigma_1}^{\sigma_2} F_\beta^{\mu\nu}(z|x) j^\beta(x)\,\mathrm{d}^4x. \qquad (13)$$

The integral on the LHS may be re-expressed by means of partial integration:

$$\left(\int_{\sigma_2} - \int_{\sigma_1}\right)\mathrm{d}\sigma_\alpha\, F_\beta^{\mu\nu}(z|x)m^{\beta\alpha}(x) - \int_{\sigma_1}^{\sigma_2}\mathrm{d}^4x\,\partial/\partial x^\alpha F_\beta^{\mu\nu}(z|x)m^{\beta\alpha}(x). \qquad (14)$$

The explicit form of F, the definition of the path $\xi(x)$, and the definition of the hyperplanes σ_1 and σ_2 lead us to the conclusion that the surface term of (14) vanishes for every point z inside the region Ω. If Ω is the whole spacetime, one can relax the assumptions on the shape of the path $\xi(x)$. In this case these can be arbitrary space-like lines. This is enough to guarantee that in the limit of $\sigma_1\to\sigma(-\infty)$ and $\sigma_2\to\sigma(+\infty)$ the surface integrals vanish for an arbitrary finite point z.

The second term of (14) can be written as follows. Using the explicit form of the kernel F, and the antisymmetry of $m^{\alpha\beta}$ we find that it is equal to

$$-\tfrac{1}{2}\int_{\sigma_1}^{\sigma_2}\mathrm{d}^4x\,\partial/\partial x^{[\alpha}\left(\int_{R(x)}^{x}\mathrm{d}\xi_{[\mu}\,\delta^{(4)}(z-\xi)\,\partial\xi_{\nu]}/\partial x^{\beta]}m^{\beta\alpha}(x)\right). \qquad (15)$$

The kernel of the integral can be rearranged in the following way

$$\partial/\partial x^{[\alpha} \int_0^1 \mathrm{d}\xi_{[\mu}/\mathrm{d}l\, \delta^{(4)}(z-\xi)\, \partial\xi_{\nu]}/\partial x^{\beta]}$$

$$= \int_0^1 \mathrm{d}l\, \partial/\partial x^{[\alpha}(\mathrm{d}\xi_{[\mu}/\mathrm{d}l)\delta^{(4)}(z-\xi)\, \partial\xi_{\nu]}/\partial x^{\beta]}$$

$$- \int_0^1 \mathrm{d}l(\mathrm{d}\xi_{[\mu}/\mathrm{d}l)(\partial\xi^{\gamma}/\partial x^{[\alpha})\, \partial/\partial z^{\gamma}\delta^{(4)}(z-\xi)(\partial\xi_{\nu]}/\partial x^{\beta]}). \qquad (16)$$

Combining the symmetry properties of this expression, and the relation

$$(\partial\xi_{[\mu}(x,l)/\partial x^{[\alpha})(\partial\xi_{\nu]}(x,l)/\partial x^{\beta]})|_{l=0} = \partial R_{[\mu}/\partial x^{[\alpha}\, \partial R_{\nu]}/\partial x^{\beta]}, \qquad (17)$$

after partial integration the first term on the RHS of (16) reads

$$+\tfrac{1}{2}g_{\mu[\alpha}g_{\beta]\nu}\delta^{(4)}(z-x) - \tfrac{1}{2}g_{\nu[\alpha}g_{\beta]\mu}\delta^{(4)}(z-x)$$

$$-\tfrac{1}{2}\int_0^1 \mathrm{d}l\, \partial\xi_{[\mu}/\partial x^{[\alpha}\, \mathrm{d}\xi^{\gamma}/\mathrm{d}l\, \partial/\partial z^{\gamma}\delta^{(4)}(z-\xi)\, \partial\xi_{\nu]}/\partial x^{\beta]}. \qquad (18)$$

Finally, the equation (13) implies that $m^{\alpha\beta}$ has the general form

$$m^{\nu\mu}(z) = \int_{\sigma_1}^{\sigma_2} F_{\rho}^{\mu\nu}(z|x)j^{\rho}(x)\,\mathrm{d}^4x$$

$$-\partial/\partial z^{\gamma}\left(\tfrac{1}{2}\int_{\sigma_1}^{\sigma_2} \mathrm{d}^4x[A_{\alpha\beta}^{\mu\gamma\nu}(z|x) - A_{\alpha\beta}^{\nu\gamma\mu}(z|x) - A_{\alpha\beta}^{\gamma\mu\nu}(z|x)]m^{\beta\alpha}(x)\right), \qquad (19)$$

where

$$A_{\alpha\beta}^{\mu\gamma\nu}(z|x) = \int_0^1 \mathrm{d}\xi^{\mu}(x,l)/\mathrm{d}l\, \partial\xi^{\gamma}/\partial x^{[\alpha}\delta^{(4)}(z-\xi)\, \partial\xi^{\nu}/\partial x^{\beta]}. \qquad (20)$$

Using the properties of the pseudotensor $\epsilon^{\mu\nu\gamma\delta}$ one can express (19) as

$$m^{\mu\nu}(z) = \int_{\sigma_1}^{\sigma_2} F_{\beta}^{\mu\nu}(z|x)j^{\beta}(x)\,\mathrm{d}^4x + \partial/\partial z^{\gamma}[\epsilon^{\mu\nu\gamma\delta}\chi_{\delta}(z)] \qquad (21)$$

where

$$\chi_{\delta}(z) = \tfrac{1}{2}\int_{\sigma_1}^{\sigma_2} \mathrm{d}^4x\, \epsilon_{\delta\epsilon\zeta\eta}A^{\epsilon\zeta\eta}{}_{\alpha\beta}(z|x)m^{\alpha\beta}(x). \qquad (22)$$

This leads to the conclusion that the general solution of (3) is the sum of the special solution of (8) and the general solution of the homogeneous equation (12).

We may ask now about the explicit form of the polarisation and magnetisation fields defined by (8). In the privileged reference frame these read

$$p^i(z) = m^{i0}(z) = \int \mathrm{d}^3x \int_0^1 \mathrm{d}l\, \mathrm{d}\xi^i(x,l)/\mathrm{d}l\, \delta^{(3)}[z-\xi(x,l)]j^0(x,z_0), \qquad (23)$$

and

$$m^i(z) = \tfrac{1}{2}\epsilon^{ijk}m^{jk}(z)$$

$$= \int \mathrm{d}^3x \int_0^1 \mathrm{d}l\, \epsilon^{ijk}\, \mathrm{d}\xi^j/\mathrm{d}l\, \partial\xi^k/\partial x^{\rho}\, \delta^{(3)}[z-\xi(x,l)]j^{\rho}(x,z_0). \qquad (24)$$

If the lines in (8) do not evolve with time, or in other words if $\partial\xi^k/\partial x^0=0$ in the privileged reference frame, than we have

$$m^i(z)=\int d^3x \int_0^1 dl\, \epsilon^{ijk}\, d\xi^j/dl\, \partial\xi^k/\partial x^m\, \delta^{(3)}[z-\xi(x,l)]j^m(x,z_0). \qquad (25)$$

The equations (23) and (25) are generalisations of the formulae by Babiker (1975).

3. Action integral

Here we study the interaction term of the action integral of electrodynamics. It will be shown that the action integral, in which electromagnetic potentials a_μ are linked to the current four-vector in a local interaction term of the form

$$\int_{\sigma_1}^{\sigma_2} j^\mu a_\mu\, d^4x \qquad (26)$$

can be rewritten in a non-local, path-dependent, but gauge-invariant form with the interaction Lagrangian given by (1). For the case of point particles this has been shown in the papers of Fiutak and Żukowski (1978) and Healy (1980). The non-relativistic case has been studied in many works, e.g. Woolley (1975a, b), Healy (1979). Here, the case of spinor electrodynamics will be given as an illustration of this general property.

The action integral for the theory is given by

$$W=-\int_{\sigma_1}^{\sigma_2} d^4x(\bar\psi\gamma^\mu\partial_\mu\psi+m\bar\psi\psi+\mathrm{i}e\bar\psi\gamma^\mu a_\mu\psi+\tfrac{1}{4}f_{\mu\nu}f^{\mu\nu}). \qquad (27)$$

One can introduce a new spinor field $\psi_p(x)$, defined by

$$\psi_p(x)=\psi(x)\exp\left(\mathrm{i}e\int_{R(x)}^{x} d\xi^\mu\, a_\mu(\xi)\right). \qquad (28)$$

The paths in (28) are defined in such a way, that when x belongs to σ_1 or σ_2, the whole path lies entirely in the respective hypersurface. With the use of the identity

$$\partial/\partial x^\mu \int_{R(x)}^{x} a_\sigma(\xi)\, d\xi^\sigma$$
$$=-\int_{R(x)}^{x} d\xi^\alpha\, \partial\xi^\gamma/\partial x^\mu f_{\alpha\sigma}(\xi)+a_\mu(x)-a_\sigma(R(x))\,\partial R^\sigma(x)/\partial x^\mu \qquad (29)$$

one can obtain

$$W=-\int_{\sigma_1}^{\sigma_2} d^4x\left(\bar\psi_p\gamma^\mu\partial_\mu\psi_p+m\bar\psi_p\psi_p+\mathrm{i}e\bar\psi_p(x)\gamma^\mu\int_{R(x)}^{x} d\xi^\alpha\, \partial\xi^\sigma/\partial x^\mu\right.$$
$$\left.\times f_{\alpha\beta}(\xi)\psi_p(x)+\mathrm{i}e\bar\psi_p(x)\gamma^\mu a_\sigma(x)\,\partial R^\sigma(x)/\partial x^\mu\psi_p(x)+\tfrac{1}{4}f_{\mu\nu}f^{\mu\nu}\right). \qquad (30)$$

The identity (29) can be easily proven if one first parametrises the path ξ^σ, then performs the differentiation, and finally integrates by parts one of the resulting expressions.

Since the tensor $f_{\alpha\beta}$ is an antisymmetric one, one can rewrite the third term of (29) in the form of the expression (1) with $m^{\alpha\beta}$ given by

$$m^{\alpha\beta}(x) = -\int_{\sigma_1}^{\sigma_2} F^{\alpha\beta}_{\rho}(x|z)(\mathrm{i}e\bar{\psi}_p(z)\gamma^{\rho}\psi_p(z))\, d^4z. \tag{31}$$

The last term of (30) vanishes. In the reference frame where $\partial R^{\alpha}/\partial x^{\mu}$ has the properties (7), it is equal to

$$\int_{x_1^0}^{x_2^0} \mathrm{d}x^0 \int \mathrm{d}\sigma_0[-\mathrm{i}e\bar{\psi}_p(x, x^0)\gamma_0\psi_p(x, x^0)a_0(R, x^0)]$$
$$= \int_{x_1^0}^{x_2^0} \mathrm{d}x^0\, a_0(R, x^0) \int \mathrm{d}^3x[-\mathrm{i}e\bar{\psi}_p(x, x^0)\gamma_0\psi(x, x^0)]. \tag{32}$$

Since the point R is fixed, $a^0(R, x^0)$ depends only upon the x^0 coordinate. The total charge carried by the spinor field is zero (5). Thus (32) vanishes.

The new action integral,

$$W = -\int_{\sigma_1}^{\sigma_2} \mathrm{d}^4x(\bar{\psi}_p\gamma^{\mu}\partial_{\mu}\psi_p + m\bar{\psi}_p\psi_p - \tfrac{1}{2}f_{\mu\nu}(x)m^{\mu\nu}(x) + \tfrac{1}{4}f_{\mu\nu}f^{\mu\nu}), \tag{33}$$

yields equivalent equations of motion for the system. As ψ_p is defined by (28), the assumption that $\delta\psi(x)$ and $\delta a_{\mu}(x)$ are vanishing at σ_1 and σ_2 is sufficient for $\delta\psi_p$ to vanish there.

The task of rewriting W in the form (33) can also be accomplished by a gauge transformation

$$a'_{\mu}(x) = a_{\mu}(x) - \partial/\partial x^{\mu} \int_{R(x)}^{x} \mathrm{d}\xi^{\alpha}\, a_{\alpha}(\xi), \tag{34}$$

or by adding to W an additional term, which describes the interaction with a compensating current (Białynicki-Birula and Białynicka-Birula 1974, Fiutak and Żukowski 1978, Woolley 1980).

Acknowledgment

This work has been supported by the Ministerstwo Szkolnictwa Wyższego, Nauki i Techniki, Project MR.I.7.

References

Babiker M 1975 *Proc. R. Soc.* A **342** 113
Babiker M, Power E A and Thirunamachandran T 1973 *Proc. R. Soc.* A **332** 187
—— 1974 *Proc. R. Soc.* A **338** 235
Białynicki-Birula I and Białynicka-Birula Z 1974 *Quantum Electrodynamics* (Oxford: Pergamon)
de Groot S R 1969 *Maxwell Equations* (Amsterdam: North-Holland)
de Groot S R and Suttorp L G 1972 *Foundations of Electrodynamics* (Amsterdam: North-Holland)
Fiutak J and Żukowski M 1978 *Acta Phys. Pol.* A **54** 533
Healy W P 1977 *Proc. R. Soc.* A **358** 367
—— 1978 *J. Phys. A: Math. Gen.* **11** 1899
—— 1979 *Phys. Rev.* A **19** 2353
—— 1980 *J. Phys. A: Math. Gen.* **13** 2383

Power E A and Thirunamachandran T 1971 *Mathematika* **18** 240
Power E A and Zienau S 1957 *Nuovo Cimento* **6** 7
—— 1959 *Phil. Trans. R. Soc.* A **251** 427
Woolley R G 1971 *Proc. R. Soc.* A **321** 551
—— 1975a *Ann. Inst. H. Poincaré* **23** 365
—— 1975b *Adv. Chem. Phys.* **33** 153
—— 1980 *J. Phys. A: Math. Gen.* **13** 2795