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Abstract. In the minimal-coupling Lagrangian for the interaction of the electromagnetic field and non-relativistic charged particles, the charge and current densities are coupled to scalar and vector potentials. In the multipolar Lagrangian, on the other hand, the aggregate or particles is partially (though sometimes completely) described by polarisation and magnetisation fields and these are coupled to the electric and magnetic induction fields. It is shown that if isotropically averaged polarisation and magnetisation fields are introduced, the minimal-coupling and multipolar Lagrangians are identical, provided also the potentials used are those of the Coulomb gauge. The associated canonical transformation of the Hamiltonian is the identity transformation. Thus the minimal-coupling Hamiltonian can be written directly in multipolar form, without any change in the canonical dynamical variables.

1. Introduction

In this paper we consider a class of polarisation and magnetisation fields that are obtained from line-integral polarisation and magnetisation fields by isotropic averaging. The line-integral polarisation and magnetisation fields and their relation to line-integral scalar and vector potentials for the electromagnetic field have been examined in earlier papers (Healy 1977, 1979). The Lagrangian for the complete system of field and charges, when expressed in terms of path-dependent quantities coupled to path-independent quantities, is such that the minimal-coupling and multipolar interactions are the same. A similar property holds for the minimal-coupling Lagrangian in which the potentials are those of the Coulomb gauge and the multipolar Lagrangian in which the polarisation and magnetisation fields are the isotropically averaged fields introduced here—the two Lagrangians are exactly equal. This follows from the fact (Belinfante 1962) that the potentials in the Coulomb gauge are the isotropic averages of the potentials in certain of the line-integral gauges and can be expressed as volume integrals over the electric and magnetic induction fields. It is also shown that the unitary transformation of Power and Zienau (1959), which relates the minimal-coupling and multipolar forms of the Hamiltonian for the system, reduces to the identity transformation when the isotropically averaged polarisation field is used in the generating function. Thus the minimal-coupling and multipolar interaction Hamiltonians are the same and the canonical dynamical variables are unaltered. The terms linear and quadratic in the vector potential that appear in the minimal-coupling form of the interaction Hamiltonian correspond, exactly and respectively, to the magnetisation and diamagnetisation terms that appear in the multipolar form. There is no coupling between the isotropically averaged polarisation field and the transverse electric field, as the former is purely longitudinal.

2. Polarisation and magnetisation fields

The system to be considered consists of a finite number of slowly moving charged point particles in interaction with the electromagnetic field. If particle α has charge e_α and position vector $\boldsymbol{q}_\alpha$, then the charge and current densities at the field point $\boldsymbol{r}$ and the time t are given by

$$\rho(\boldsymbol{r}, t) = \sum_\alpha e_\alpha \delta(\boldsymbol{r} - \boldsymbol{q}_\alpha), \tag{1}$$

$$\boldsymbol{j}(\boldsymbol{r}, t) = \sum_\alpha e_\alpha \dot{\boldsymbol{q}}_\alpha \delta(\boldsymbol{r} - \boldsymbol{q}_\alpha), \tag{2}$$

where the dot denotes differentiation with respect to t and δ is the three-dimensional Dirac delta function. The charge and current densities ρ and $\boldsymbol{j}$ satisfy the continuity or charge conservation equation

$$\nabla \cdot \boldsymbol{j} + \dot{\rho} = 0. \tag{3}$$

We introduce a reference point $\boldsymbol{R}$ which need not coincide with a material particle but may move with the aggregate as a whole. ($\boldsymbol{R}$ could be, for instance, the centre of mass.) The 'true' charge and current densities associated with this reference point are defined by

$$\rho_{\text{true}}(\boldsymbol{r}, t) = Q\delta(\boldsymbol{r} - \boldsymbol{R}), \tag{4}$$

$$\boldsymbol{j}_{\text{true}}(\boldsymbol{r}, t) = Q\dot{\boldsymbol{R}}\delta(\boldsymbol{r} - \boldsymbol{R}), \tag{5}$$

where Q is the total charge of the aggregate. The charge and current densities ρ and $\boldsymbol{j}$ are sources for the microscopic electric field $\boldsymbol{e}$ and magnetic induction field $\boldsymbol{b}$,

$$\nabla \cdot \boldsymbol{e} = 4\pi\rho, \tag{6}$$

$$\nabla \times \boldsymbol{b} = (4\pi/c)\boldsymbol{j} + (1/c)\dot{\boldsymbol{e}}, \tag{7}$$

whereas the true charge and current densities ρ_{true} and $\boldsymbol{j}_{\text{true}}$ are sources for the microscopic electric displacement vector $\boldsymbol{d}$ and magnetic field $\boldsymbol{h}$,

$$\nabla \cdot \boldsymbol{d} = 4\pi\rho_{\text{true}}, \tag{8}$$

$$\nabla \times \boldsymbol{h} = (4\pi/c)\boldsymbol{j}_{\text{true}} + (1/c)\dot{\boldsymbol{d}}. \tag{9}$$

The fields are interrelated through the equations

$$\boldsymbol{d} = \boldsymbol{e} + 4\pi\boldsymbol{p}, \tag{10}$$

$$\boldsymbol{h} = \boldsymbol{b} - 4\pi\boldsymbol{m}, \tag{11}$$

where $\boldsymbol{p}$ and $\boldsymbol{m}$ are microscopic polarisation and magnetisation fields and must satisfy

$$\tilde{\rho} \equiv \rho - \rho_{\text{true}} = -\nabla \cdot \boldsymbol{p}, \tag{12}$$

$$\tilde{\boldsymbol{j}} \equiv \boldsymbol{j} - \boldsymbol{j}_{\text{true}} = \dot{\boldsymbol{p}} + c\nabla \times \boldsymbol{m}. \tag{13}$$

Here $\tilde{\rho}$ is the polarisation charge density and $\tilde{j}$ the sum of the polarisation current density and the magnetisation current density. If the system is electrically neutral ($Q = 0$) or if the reference point $\boldsymbol{R}$ is at infinity, then ρ_{true} and j_{true} vanish and $\tilde{\rho} = \rho$ and $\tilde{j} = j$. We note that ρ_{true} and j_{true}, and hence $\tilde{\rho}$ and $\tilde{j}$, satisfy the continuity equation just like ρ and j.

2.1. Line-integral solutions

Particular polarisation and magnetisation fields having the form of line integrals have been given previously (Healy 1977). For each instant of time and for each particle α we choose a smoothly varying curve C_α starting at $\boldsymbol{R}$ and ending at $\boldsymbol{q}_\alpha$. Then

$$\boldsymbol{p}(\boldsymbol{r}, t) = \sum_\alpha e_\alpha \int_{C_\alpha} \mathrm{d}\boldsymbol{r}'\, \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{14}$$

and

$$\boldsymbol{m}(\boldsymbol{r}, t) = \sum_\alpha (e_\alpha / c) \int_{C_\alpha} \mathrm{d}\boldsymbol{r}' \times \dot{\boldsymbol{r}}' \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{15}$$

define solutions of equations (12) and (13). A physical interpretation of these fields can be given in terms of the virtual displacement of all the charges from their actual positions to the reference point and the formation of compensating electric and magnetic dipoles distributed along the integration paths (Healy 1982).

A special class of integration paths will be of interest to us here. Let C_α consist of a pair of parallel straight lines, one starting at $\boldsymbol{R}$ and extending to infinity in the direction specified by a unit vector $\hat{\boldsymbol{\varepsilon}}$ and the other coming from infinity in the direction of $-\hat{\boldsymbol{\varepsilon}}$ and ending at the charge position $\boldsymbol{q}_\alpha$. The vector $\hat{\boldsymbol{\varepsilon}}$ is to be time independent and the same for all α. The polarisation and magnetisation fields associated with these integration paths may then be denoted by $\boldsymbol{p}(\boldsymbol{r}, t, \hat{\boldsymbol{\varepsilon}})$ and $\boldsymbol{m}(\boldsymbol{r}, t, \hat{\boldsymbol{\varepsilon}})$, respectively. We introduce a real parameter u for the outward portion of C_α (which is common to all the charges), so that a point on this portion is given by

$$\boldsymbol{r}' = \boldsymbol{R} + u\hat{\boldsymbol{\varepsilon}}, \qquad 0 \leqslant u < \infty, \tag{16}$$

and a real parameter u_α for the inward portion, so that a point on this portion is given by

$$\boldsymbol{r}' = \boldsymbol{q}_\alpha + u_\alpha \hat{\boldsymbol{\varepsilon}}, \qquad \infty > u_\alpha \geqslant 0. \tag{17}$$

Using these parameters, we obtain for the straight-line polarisation and magnetisation fields

$$\boldsymbol{p}(\boldsymbol{r}, t, \hat{\boldsymbol{\varepsilon}}) = Q \int_0^\infty \hat{\boldsymbol{\varepsilon}} \delta(\boldsymbol{r} - \boldsymbol{r}')\, \mathrm{d}u - \sum_\alpha e_\alpha \int_0^\infty \hat{\boldsymbol{\varepsilon}} \delta(\boldsymbol{r} - \boldsymbol{r}')\, \mathrm{d}u_\alpha \tag{18}$$

and

$$\boldsymbol{m}(\boldsymbol{r}, t, \hat{\boldsymbol{\varepsilon}}) = \frac{Q}{c} \int_0^\infty \hat{\boldsymbol{\varepsilon}} \times \dot{\boldsymbol{R}} \delta(\boldsymbol{r} - \boldsymbol{r}')\, \mathrm{d}u - \sum_\alpha \frac{e_\alpha}{c} \int_0^\infty \hat{\boldsymbol{\varepsilon}} \times \dot{\boldsymbol{q}}_\alpha \delta(\boldsymbol{r} - \boldsymbol{r}')\, \mathrm{d}u_\alpha. \tag{19}$$

2.2. Isotropic averaging

The polarisation and magnetisation fields of equations (18) and (19) still depend on the direction of the vector $\hat{\boldsymbol{\varepsilon}}$. This dependence may be eliminated by performing an unweighted averaging over all directions. The isotropically averaged fields will also be valid polarisation and magnetisation fields, since the right-hand sides of the inhomogeneous defining equations (12) and (13) are linear in $\boldsymbol{p}$ and $\boldsymbol{m}$. Now on the outward portion of C_α

$$u = |\boldsymbol{r}' - \boldsymbol{R}| \qquad \text{and} \qquad \hat{\boldsymbol{\varepsilon}} = (\boldsymbol{r}' - \boldsymbol{R})/|\boldsymbol{r}' - \boldsymbol{R}|, \tag{20}$$

while on the inward portion

$$u_\alpha = |\boldsymbol{r}' - \boldsymbol{q}_\alpha| \qquad \text{and} \qquad \hat{\boldsymbol{\varepsilon}} = (\boldsymbol{r}' - \boldsymbol{q}_\alpha)/|\boldsymbol{r}' - \boldsymbol{q}_\alpha|. \tag{21}$$

Also, if $\mathrm{d}\Omega$ is an element of solid angle about the direction of $\hat{\boldsymbol{\varepsilon}}$, the differential volume element may be expressed as

$$\mathrm{d}^3 r' = u^2 \,\mathrm{d}u \,\mathrm{d}\Omega \tag{22}$$

with $\boldsymbol{R}$ as origin of a spherical polar coordinate system or as

$$\mathrm{d}^3 r' = u_\alpha^2 \,\mathrm{d}u_\alpha \,\mathrm{d}\Omega \tag{23}$$

with $\boldsymbol{q}_\alpha$ as origin. It follows from this and equations (18) and (19) that the isotropically averaged fields are given by

$$\boldsymbol{p}(\boldsymbol{r}, t) \equiv \frac{1}{4\pi} \oiint \boldsymbol{p}(\boldsymbol{r}, t, \hat{\boldsymbol{\varepsilon}}) \,\mathrm{d}\Omega = \frac{1}{4\pi}\left(Q\frac{\boldsymbol{r} - \boldsymbol{R}}{|\boldsymbol{r} - \boldsymbol{R}|^3} - \sum_\alpha e_\alpha \frac{\boldsymbol{r} - \boldsymbol{q}_\alpha}{|\boldsymbol{r} - \boldsymbol{q}_\alpha|^3}\right) \tag{24}$$

and

$$\boldsymbol{m}(\boldsymbol{r}, t) \equiv \frac{1}{4\pi} \oiint \boldsymbol{m}(\boldsymbol{r}, t, \hat{\boldsymbol{\varepsilon}}) \,\mathrm{d}\Omega = \frac{1}{4\pi}\left(\frac{Q}{c}\frac{(\boldsymbol{r} - \boldsymbol{R}) \times \dot{\boldsymbol{R}}}{|\boldsymbol{r} - \boldsymbol{R}|^3} - \sum_\alpha \frac{e_\alpha}{c} \frac{(\boldsymbol{r} - \boldsymbol{q}_\alpha) \times \dot{\boldsymbol{q}}_\alpha}{|\boldsymbol{r} - \boldsymbol{q}_\alpha|^3}\right). \tag{25}$$

Here the properties of the Dirac delta function have been used to reduce the volume integrals over all space. If these integrals are left intact, we may express the isotropically averaged fields as

$$\boldsymbol{p}(\boldsymbol{r}, t) = \frac{1}{4\pi} \iiint \frac{(\boldsymbol{r}' - \boldsymbol{r})\tilde{\rho}(\boldsymbol{r}', t)}{|\boldsymbol{r}' - \boldsymbol{r}|^3} \mathrm{d}^3 r' = \frac{1}{4\pi} \iiint \frac{\nabla' \tilde{\rho}(\boldsymbol{r}', t)}{|\boldsymbol{r}' - \boldsymbol{r}|} \mathrm{d}^3 r' \tag{26}$$

and

$$\boldsymbol{m}(\boldsymbol{r}, t) = \frac{1}{4\pi c} \iiint \frac{(\boldsymbol{r}' - \boldsymbol{r}) \times \tilde{\boldsymbol{j}}(\boldsymbol{r}', t)}{|\boldsymbol{r}' - \boldsymbol{r}|^3} \mathrm{d}^3 r' = \frac{1}{4\pi c} \iiint \frac{\nabla' \times \tilde{\boldsymbol{j}}(\boldsymbol{r}', t)}{|\boldsymbol{r}' - \boldsymbol{r}|} \mathrm{d}^3 r' \tag{27}$$

where the second forms are obtained from the first by using integration by parts and the fact that both $\tilde{\rho}$ and $\tilde{\boldsymbol{j}}$ vanish for r sufficiently large. The integral expressions (26) and (27) apply to a continuous as well as to a discrete distribution, provided the bound charge and current densities satisfy the continuity equation and vanish sufficiently rapidly at infinity (see appendix 1). It should be noted that the isotropically averaged polarisation and magnetisation fields are, apart from constant factors, the electric and magnetic induction fields that would arise, according to the Coulomb and Biot–Savart laws, from a static charge density $\tilde{\rho}$ and a stationary current density $\tilde{\boldsymbol{j}}$. We emphasise, however, that despite their 'instantaneous' character, these fields are exact solutions of the simultaneous time-dependent equations (12) and (13).

3. Lagrangian

The minimal-coupling Lagrangian for the electromagnetic field interacting with non-relativistic charged point particles is represented as a sum of gauge-independent and gauge-dependent parts by

$$L = L_0 + L_1 \tag{28}$$

where

$$L_0 = \frac{1}{8\pi}\iiint (e^2 - b^2)\, d^3r + \tfrac{1}{2}\sum_\alpha m_\alpha \dot{q}_\alpha^2 \tag{29}$$

and

$$L_1 = \iiint [(1/c)\boldsymbol{j}\cdot\boldsymbol{a} - \rho\phi]\, d^3r. \tag{30}$$

The microscopic electric and magnetic induction fields $\boldsymbol{e}$ and $\boldsymbol{b}$ are derived from the potentials ϕ and $\boldsymbol{a}$ through the equations

$$\boldsymbol{e} = -\nabla\phi - (1/c)\dot{\boldsymbol{a}}, \tag{31}$$

$$\boldsymbol{b} = \nabla \times \boldsymbol{a}, \tag{32}$$

and m_α is the mass of particle α. Changing the potentials in L_1 through a gauge transformation for which the gauge function involves the Lagrangian coordinates alone yields an equivalent Lagrangian that differs from L only by the addition of a total time derivative of a function or functional of the coordinates. We here take the potentials to be those of the Coulomb gauge, with the variations of $\boldsymbol{a}$ in Hamilton's principle being restricted by the transversality condition and with ϕ being regarded, not as a dynamical variable of the field, but as a prescribed function of the particle coordinates. Thus (Belinfante 1962)

$$\phi(\boldsymbol{r}, t) = \frac{1}{4\pi}\iiint \frac{(\boldsymbol{r}' - \boldsymbol{r})\cdot\boldsymbol{e}(\boldsymbol{r}', t)}{|\boldsymbol{r}' - \boldsymbol{r}|^3}\, d^3r' = \frac{1}{4\pi}\iiint \frac{\nabla'\cdot\boldsymbol{e}(\boldsymbol{r}', t)}{|\boldsymbol{r}' - \boldsymbol{r}|}\, d^3r' \tag{33}$$

and

$$\boldsymbol{a}(\boldsymbol{r}, t) = \frac{1}{4\pi}\iiint \frac{(\boldsymbol{r}' - \boldsymbol{r})\times\boldsymbol{b}(\boldsymbol{r}', t)}{|\boldsymbol{r}' - \boldsymbol{r}|^3}\, d^3r' = \frac{1}{4\pi}\iiint \frac{\nabla'\times\boldsymbol{b}(\boldsymbol{r}', t)}{|\boldsymbol{r}' - \boldsymbol{r}|}\, d^3r'. \tag{34}$$

The first forms are obtained by an isotropic averaging of the potentials in those line-integral gauges for which the integration paths consist of fixed parallel straight lines coming from infinity and ending at the field points, and the second forms follow from them through integration by parts. Since $\nabla\cdot\boldsymbol{e} = 4\pi\rho$, the scalar potential may be written as

$$\phi(\boldsymbol{r}, t) = \iiint \frac{\rho(\boldsymbol{r}', t)}{|\boldsymbol{r}' - \boldsymbol{r}|}\, d^3r' = \sum_\alpha \frac{e_\alpha}{|\boldsymbol{q}_\alpha - \boldsymbol{r}|} \tag{35}$$

which shows that ϕ is the instantaneous electrostatic or Coulomb potential of the point charges. It may also be shown, by differentiating with respect to $\boldsymbol{r}$ under the integral sign, that $\nabla\cdot\boldsymbol{a} = 0$, so that the Coulomb gauge condition is satisfied.

Splitting the charge and current densities into true and bound contributions as in equations (12) and (13), we express the interaction Lagrangian (30) as

$$L_1 = (Q/c)\dot{\boldsymbol{R}} \cdot \boldsymbol{a}(\boldsymbol{R}, t) - Q\phi(\boldsymbol{R}, t) + \iiint [(1/c)\tilde{\boldsymbol{j}} \cdot \boldsymbol{a} - \tilde{\rho}\phi]\, \mathrm{d}^3 r. \tag{36}$$

The first two terms correspond to the interaction Lagrangian for a collective particle of charge Q moving with the reference point in the field described by the Coulomb potentials ϕ and $\boldsymbol{a}$. They vanish if the system is neutral ($Q = 0$) or if $\boldsymbol{R}$ is at infinity (where ϕ and $\boldsymbol{a}$ are zero). In the remaining terms of equation (36) we insert the formulae (33) and (34) for the potentials, invert the order of integration and interchange the roles of the dummy variables $\boldsymbol{r}$ and $\boldsymbol{r}'$. We then obtain

$$L_1 = (Q/c)\dot{\boldsymbol{R}} \cdot \boldsymbol{a}(\boldsymbol{R}, t) - Q\phi(\boldsymbol{R}, t) + \iiint (\boldsymbol{p} \cdot \boldsymbol{e} + \boldsymbol{m} \cdot \boldsymbol{b})\, \mathrm{d}^3 r \tag{37}$$

where $\boldsymbol{p}$ and $\boldsymbol{m}$ are defined by (24) and (25). This is just the multipolar interaction Lagrangian associated with these polarisation and magnetisation fields. Thus when the isotropically averaged polarisation and magnetisation fields are used, the multipolar and minimal-coupling Lagrangians are identical, provided the potentials are those of the Coulomb gauge.

4. Hamiltonian

The quantum mechanical interaction energy operator that results from the minimal-coupling substitution $\boldsymbol{p}_\alpha \to \boldsymbol{p}_\alpha - (e_\alpha/c)\boldsymbol{a}(\boldsymbol{q}_\alpha)$ in the Hamiltonian for the uncoupled systems is given by

$$H_{\mathrm{int}} = -\sum_\alpha (e_\alpha/m_\alpha c)\boldsymbol{p}_\alpha \cdot \boldsymbol{a}(\boldsymbol{q}_\alpha) + \sum_\alpha (e_\alpha^2/2m_\alpha c^2)\boldsymbol{a}^2(\boldsymbol{q}_\alpha). \tag{38}$$

Here $\boldsymbol{p}_\alpha$ is the canonical momentum conjugate to $\boldsymbol{q}_\alpha$ and $\boldsymbol{a}(\boldsymbol{r})$ is the vector potential in the Coulomb gauge. (As the notation indicates, we are using the Schrödinger picture of the motion.) Because $\boldsymbol{a}$ is transverse, the order of the operators $\boldsymbol{p}_\alpha$ and $\boldsymbol{a}(\boldsymbol{q}_\alpha)$ in H_{int} is immaterial. The minimal-coupling Hamiltonian may be changed to multipolar form by means of the unitary operator $\exp(\mathrm{i}W/\hbar)$ in which the generating function is defined by

$$W = (1/c)\iiint \boldsymbol{p} \cdot \boldsymbol{a}\, \mathrm{d}^3 r \tag{39}$$

where $\boldsymbol{p}$ is a polarisation field for the aggregate of particles. Previously the multipolar Hamiltonian has been derived by using the line-integral polarisation field (14) in W (see e.g. Healy 1982). We can also, however, use the isotropically averaged polarisation field (24). Now this field is purely longitudinal—it is the longitudinal part of *any* polarisation field associated with the reference point $\boldsymbol{R}$, as all these fields differ only in their transverse parts (Woolley 1975, Healy 1977). Since also the vector potential in the Coulomb gauge is purely transverse, the generating function W vanishes and the unitary operator defining the canonical transformation is just the identity:

$$W = (1/c)\iiint \boldsymbol{p}^{\parallel} \cdot \boldsymbol{a}^{\perp}\, \mathrm{d}^3 r = 0, \qquad \exp(\mathrm{i}W/\hbar) = 1. \tag{40}$$

Nevertheless, there is a multipolar form of the Hamiltonian corresponding to this polarisation field, as we shall now verify. For simplicity, we take the reference point $\boldsymbol{R}$ to be fixed.

Substituting from the first of the formulae (34) for the vector potential as a volume integral over the magnetic induction field gives immediately

$$-\sum_\alpha (e_\alpha/m_\alpha c)\boldsymbol{p}_\alpha \cdot \boldsymbol{a}(\boldsymbol{q}_\alpha) = -\iiint \tilde{\boldsymbol{m}}(\boldsymbol{r}) \cdot \boldsymbol{b}(\boldsymbol{r})\,\mathrm{d}^3r \tag{41}$$

with

$$\tilde{\boldsymbol{m}}(\boldsymbol{r}) = \frac{1}{4\pi}\sum_\alpha \frac{e_\alpha}{m_\alpha c}\frac{(\boldsymbol{q}_\alpha - \boldsymbol{r})\times \boldsymbol{p}_\alpha}{|\boldsymbol{q}_\alpha - \boldsymbol{r}|^3}. \tag{42}$$

The magnetisation field $\tilde{\boldsymbol{m}}$ in the Hamiltonian is obtained from the magnetisation field $\boldsymbol{m}$ in the Lagrangian through the usual prescription—the physical momenta of the particles are replaced by the corresponding transformed canonical momenta. It should be noted that in the present case (i) the reference point is fixed, (ii) since the transformation is the identity, the new canonical momenta are the same as the old and (iii) the magnetisation fields do not have to be symmetrised to make them Hermitian, as angular momentum operators commute with isotropic functions of the coordinates. The same substitution for the vector potential also gives

$$\sum_\alpha (e_\alpha^2/2m_\alpha c^2)\boldsymbol{a}^2(\boldsymbol{q}_\alpha) = \tfrac{1}{2}\iiint \mathrm{d}^3r \iiint \mathrm{d}^3s\, o_{ij}(\boldsymbol{r}, \boldsymbol{s}) b_i(\boldsymbol{r}) b_j(\boldsymbol{s}) \tag{43}$$

where o is a diamagnetisation tensor field defined by

$$o_{ij}(\boldsymbol{r}, \boldsymbol{s}) = \frac{1}{(4\pi)^2}\sum_\alpha \frac{e_\alpha^2}{m_\alpha c^2}\frac{(\boldsymbol{q}_\alpha - \boldsymbol{r})\cdot(\boldsymbol{q}_\alpha - \boldsymbol{s})\delta_{ij} - (\boldsymbol{q}_\alpha - \boldsymbol{r})_j \cdot (\boldsymbol{q}_\alpha - \boldsymbol{s})_i}{|\boldsymbol{q}_\alpha - \boldsymbol{r}|^3 |\boldsymbol{q}_\alpha - \boldsymbol{s}|^3}. \tag{44}$$

It is shown in appendix 2 that this field too may be obtained by isotropic averaging. Moreover, it follows readily from the relation

$$m_\alpha \dot{\boldsymbol{q}}_\alpha = \boldsymbol{p}_\alpha - (e_\alpha/c)\boldsymbol{a}(\boldsymbol{q}_\alpha) \tag{45}$$

that the istropically averaged fields, just like the line-integral fields, satisfy

$$m_i(\boldsymbol{r}) = \tilde{m}_i(\boldsymbol{r}) - \iiint o_{ij}(\boldsymbol{r}, \boldsymbol{s}) b_j(\boldsymbol{s})\,\mathrm{d}^3s. \tag{46}$$

Combination of (41) and (43) enables the minimal-coupling interaction Hamiltonian (38) to be written in typical multipolar form:

$$H_{\mathrm{int}} = -\iiint \tilde{\boldsymbol{m}}(\boldsymbol{r}) \cdot \boldsymbol{b}(\boldsymbol{r})\,\mathrm{d}^3r + \tfrac{1}{2}\iiint \mathrm{d}^3r \iiint \mathrm{d}^3s\, o_{ij}(\boldsymbol{r}, \boldsymbol{s}) b_i(\boldsymbol{r}) b_j(\boldsymbol{s}). \tag{47}$$

The electric interaction term $-\iiint \boldsymbol{p} \cdot \boldsymbol{d}^\perp\,\mathrm{d}^3r$ (where $\boldsymbol{d}$ is the microscopic displacement vector $\boldsymbol{e} + 4\pi\boldsymbol{p}$) and the self-energy term $2\pi\iiint \boldsymbol{p}^{\perp 2}\,\mathrm{d}^3r$, which occur when the line-integral polarisation field is used, both vanish here because the isotropically averaged polarisation field is purely longitudinal. We emphasise that equations (38) and (47) are merely two different ways of expressing the same operator H_{int} and that there is no change in either the unperturbed Hamiltonian or the canonical dynamical variables. This is in contrast to the line-integral multipolar formalism, in which the partitioning of the total Hamiltonian operator into unperturbed and interaction parts is altered and in which the field momentum conjugate to $\boldsymbol{a}$ is proportional to $\boldsymbol{d}^{\perp}$ rather than to $\boldsymbol{e}^{\perp}$.

5. Summary

The polarisation and magnetisation fields discussed in § 2 are the unweighted averages of the path-dependent polarisation and magnetisation fields taken over all straight-line integration paths ending at the positions of the charged particles. It is shown in appendix 1 that the integral expressions for these fields apply to a continuous as well as to a discrete distribution of charge and current densities. The equality of the minimal-coupling and multipolar interactions was demonstrated in § 3 for the classical Lagrangian and in § 4 for the quantum mechanical Hamiltonian. In each case the polarisation and magnetisation fields are the isotropically averaged ones and the potentials are those of the Coulomb gauge. The diamagnetisation tensor field that appears in the multipolar Hamiltonian is derived by isotropic averaging in appendix 2.

Appendix 1. Integral form of polarisation and magnetisation fields

To verify that the integral expressions (26) and (27) for the polarisation and magnetisation fields satisfy the defining equations (12) and (13), we first note that

$$-\nabla\cdot\boldsymbol{p}=-(4\pi)^{-1}\iiint\tilde{\rho}(\boldsymbol{r}',t)\nabla^2|\boldsymbol{r}-\boldsymbol{r}'|^{-1}\,\mathrm{d}^3r'=\tilde{\rho}(\boldsymbol{r},t), \tag{A1.1}$$

as required. Here we have used the representation

$$\delta(\boldsymbol{r})=-(1/4\pi)\nabla^2(1/r) \tag{A1.2}$$

of the delta function. From this representation and from the vector identity

$$\nabla\times(\boldsymbol{A}\times\boldsymbol{B})=(\boldsymbol{B}\cdot\nabla)\boldsymbol{A}-(\nabla\cdot\boldsymbol{A})\boldsymbol{B}, \tag{A1.3}$$

which applies if $\boldsymbol{B}$ is independent of $\boldsymbol{r}$, it follows that

$$c\nabla\times\boldsymbol{m}(\boldsymbol{r},t)=\tilde{\boldsymbol{j}}(\boldsymbol{r},t)+(4\pi)^{-1}\iiint\{\tilde{\boldsymbol{j}}(\boldsymbol{r}',t)\cdot\nabla'\}\nabla'|\boldsymbol{r}'-\boldsymbol{r}|^{-1}\,\mathrm{d}^3r'. \tag{A1.4}$$

Since $\tilde{\rho}$ and $\tilde{\boldsymbol{j}}$ are assumed to satisfy the continuity equation, we also have

$$\begin{aligned}\dot{\boldsymbol{p}}(\boldsymbol{r},t)&=-(4\pi)^{-1}\iiint\dot{\tilde{\rho}}(\boldsymbol{r}',t)\nabla'|\boldsymbol{r}'-\boldsymbol{r}|^{-1}\,\mathrm{d}^3r'\\&=(4\pi)^{-1}\iiint\{\nabla'\cdot\tilde{\boldsymbol{j}}(\boldsymbol{r}',t)\}\nabla'|\boldsymbol{r}'-\boldsymbol{r}|^{-1}\,\mathrm{d}^3r'\\&=-(4\pi)^{-1}\iiint\{\tilde{\boldsymbol{j}}(\boldsymbol{r}',t)\cdot\nabla'\}\nabla'|\boldsymbol{r}'-\boldsymbol{r}|^{-1}\,\mathrm{d}^3r'\end{aligned} \tag{A1.5}$$

where the last line follows by integrating by parts and dropping a surface term at infinity. Addition of equations (A1.4) and (A1.5) then gives

$$\dot{p} + c\nabla \times m = \tilde{j}(r, t) \tag{A1.6}$$

and completes the verification.

Appendix 2. Isotropically averaged diamagnetisation field

The diamagnetisation tensor field of equation (44) may be derived by isotropic averaging as follows. The path-dependent diamagnetisation field (Healy 1982) is a sum of products of line integrals, namely

$$\sum_\alpha \frac{e_\alpha^2}{m_\alpha c^2} \int_{C_\alpha} \left(\mathrm{d}r' \times \frac{\partial r'}{\partial q_{\alpha k}}\right)_i \delta(r - r') \int_{C_\alpha} \left(\mathrm{d}s' \times \frac{\partial s'}{\partial q_{\alpha k}}\right)_j \delta(s - s') \tag{A2.1}$$

where the curves C_α are the same as those occurring in the path-dependent polarisation and magnetisation fields. For each particle α we now choose a pair of straight-line paths $C_\alpha(\hat{\varepsilon})$ and $C_\alpha(\hat{\eta})$ that come from infinity, end at q_α and are parallel to unit vectors $-\hat{\varepsilon}$ and $-\hat{\eta}$ respectively. With these paths we associate a tensor field defined by

$$\begin{aligned} o_{ij}(r, s, \hat{\varepsilon}, \hat{\eta}) &= \sum_\alpha \frac{e_\alpha^2}{m_\alpha c^2} \int_{C_\alpha(\hat{\varepsilon})} \left(\mathrm{d}r' \times \frac{\partial r'}{\partial q_{\alpha k}}\right)_i \delta(r - r') \int_{C_\alpha(\hat{\eta})} \left(\mathrm{d}s' \times \frac{\partial s'}{\partial q_{\alpha k}}\right)_j \delta(s - s') \\ &= \sum_\alpha \frac{e_\alpha^2}{m_\alpha c^2} \left(\delta_{ij} \int_0^\infty \hat{\varepsilon}\delta(r - r')\,\mathrm{d}u_\alpha \cdot \int_0^\infty \hat{\eta}\delta(s - s')\,\mathrm{d}v_\alpha \right. \\ &\qquad \left. - \int_0^\infty \hat{\varepsilon}_j \delta(r - r')\,\mathrm{d}u_\alpha \int_0^\infty \hat{\eta}_i \delta(s - s')\,\mathrm{d}v_\alpha \right) \end{aligned} \tag{A2.2}$$

where u_α is a parameter for $C_\alpha(\hat{\varepsilon})$ and v_α is a parameter for $C_\alpha(\hat{\eta})$. (The line-integral diamagnetisation field, for the case in which the integration paths are parallel straight lines coming from infinity, is obtained by setting $\hat{\varepsilon} = \hat{\eta}$.) If this expression is averaged over all directions of $\hat{\varepsilon}$ and $\hat{\eta}$ *independently*, then the diamagnetisation field (44) is recovered. Thus

$$\begin{aligned} &(4\pi)^{-2} \oiint\oiint o_{ij}(r, s, \hat{\varepsilon}, \hat{\eta})\,\mathrm{d}\Omega\,\mathrm{d}\Theta \\ &\quad = \frac{1}{(4\pi)^2} \sum_\alpha \frac{e_\alpha^2}{m_\alpha c^2} \frac{(q_\alpha - r)\cdot(q_\alpha - s)\delta_{ij} - (q_\alpha - r)_j (q_\alpha - s)_i}{|q_\alpha - r|^3 |q_\alpha - s|^3} \\ &\quad = o_{ij}(r, s). \end{aligned} \tag{A2.3}$$

Here $\mathrm{d}\Omega$ is an element of solid angle about $\hat{\varepsilon}$ and $\mathrm{d}\Theta$ is an element of solid angle about $\hat{\eta}$, so that, with q_α as origin, the differential volume elements in r space and s space may be expressed as

$$\mathrm{d}^3 r' = u_\alpha^2\,\mathrm{d}u_\alpha\,\mathrm{d}\Omega = |r' - q_\alpha|^2\,\mathrm{d}u_\alpha\,\mathrm{d}\Omega \tag{A2.4}$$

and

$$\mathrm{d}^3 s' = v_\alpha^2\,\mathrm{d}v_\alpha\,\mathrm{d}\Omega = |s' - q_\alpha|^2\,\mathrm{d}v_\alpha\,\mathrm{d}\Omega \tag{A2.5}$$

respectively. The properties of the Dirac delta function have again been used to reduce the volume integrals. The occurrence in equation (A2.3) of independent averages over the directions of $\hat{\varepsilon}$ and $\hat{\eta}$ was to be expected, as the diamagnetisation field arises from quadratic terms in a Hamiltonian derived from an averaged Lagrangian, and is thus composed of products of averages rather than averages of products.

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