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The multipole interaction Hamiltonian for time dependent fields

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Abstract. By a suitable choice of gauge, it is shown that the conventional Hamiltonian for the interaction of a system with time dependent electromagnetic fields can be written in multipole form without performing a canonical transformation.

1. Introduction

The Hamiltonian for the interaction of a single classical spinless particle of charge e, mass m, position $\boldsymbol{r}$, and canonical momentum $\boldsymbol{p}$ with a given electromagnetic field characterized by a vector potential $\boldsymbol{A}$ and a scalar potential ϕ is (in SI)

$$V(t) = -\frac{e}{m}\boldsymbol{p}\,.\,\boldsymbol{A}(\boldsymbol{r},t)+\frac{e^2}{2m}\boldsymbol{A}(\boldsymbol{r},t)^2+e\phi(\boldsymbol{r},t). \tag{1}$$

Our final result can be immediately quantized and extended to any number of particles; the inclusion of spin will be discussed elsewhere. It is often convenient to represent the interaction as a series of terms in which the electric and magnetic multipoles are coupled with the electric and magnetic fields and their gradients. When the fields are static, the transformation of (1) into multipole form is elementary; but when the fields are dynamic, the transformation is more difficult, and all previous treatments involve a canonical transformation of the Hamiltonian into a form which is equivalent to, but not equal to, (1). These transformations are performed either directly on the Hamiltonian, or indirectly via the corresponding Lagrangian by subtraction of a total time derivative. Complications are introduced and the simplicity of the static situation is lost.

We show that, with a more judicious choice of gauge, the interaction (1) is simply equal to the multipole Hamiltonian. This is accomplished without a canonical transformation and is almost as simple as the static case.

The original treatment of the dynamic case is due to Goeppert-Mayer (1931), who derived the electric dipole term by subtracting an appropriate total time derivative from the Lagrangian. This derivation was rediscovered by Richards (1948). The extension of this method to include the magnetic dipole and electric quadrupole terms is complicated, and was given by Shail (1964). Fiutak (1963) has attempted to derive the multipole form by a canonical transformation of the Hamiltonian; unfortunately his treatment contains some errors. Finally, we mention the discussions by Power and Zienau (1959),

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Fiutak (1963), McLachlan (1963), Shail (1964), Atkins and Woolley (1970), and Woolley (1971), who derived the multipole interactions by considering the radiation field as a dynamical system in interaction with a system of particles, rather than as a prescribed field. These treatments are more involved, but lead to additional results; for example, self-energies and binding energies.

2. Static fields

We first review the static case since this guides our explicit choice of potentials in the dynamic case. Here the electric and magnetic fields are determined by ϕ and $\boldsymbol{A}$ respectively:

$$\boldsymbol{E}(\boldsymbol{r}) = -\nabla\phi(\boldsymbol{r}) \tag{2}$$

$$\boldsymbol{B}(\boldsymbol{r}) = \nabla\times\boldsymbol{A}(\boldsymbol{r}). \tag{3}$$

By expanding $\phi(\boldsymbol{r})$ in a Taylor series about the origin,

$$\phi(\boldsymbol{r}) = \phi_0+\boldsymbol{r}\,.\,(\nabla\phi)_0+\tfrac{1}{2}\boldsymbol{rr}:(\nabla\nabla\phi)_0+\ldots, \tag{4}$$

the static electric multipole interactions are generated:

$$e\phi = e\phi_0-\boldsymbol{\mu}\,.\,\boldsymbol{E}_0-\boldsymbol{Q}:(\nabla\boldsymbol{E})_0+\ldots, \tag{5}$$

where $\boldsymbol{\mu} = e\boldsymbol{r}$ is the electric dipole moment and $\boldsymbol{Q} = \frac{1}{2}e\boldsymbol{rr}$ is the electric quadrupole moment ($\boldsymbol{Q}$ is often replaced by the traceless form $\boldsymbol{Q}-\frac{1}{6}er^2\mathbf{1}$, which is legitimate in source-free regions since $\nabla\,.\,\boldsymbol{E} = 0$). The origin is chosen to be the nucleus of an atomic charge distribution, which is assumed for simplicity to be infinitely massive compared to the electron. From the expansion

$$\boldsymbol{A}(\boldsymbol{r}) = \tfrac{1}{2}\boldsymbol{B}_0\times\boldsymbol{r}+\tfrac{1}{3}\boldsymbol{r}\,.\,(\nabla\boldsymbol{B})_0\times\boldsymbol{r}+\ldots, \tag{6}$$

which leads to the correct Taylor expansion for $\boldsymbol{B}(\boldsymbol{r})$ using (3), the static magnetic multipole interactions are derived:

$$-\frac{e}{m}\boldsymbol{p}\,.\,\boldsymbol{A} = -\boldsymbol{m}\,.\,\boldsymbol{B}_0+\ldots, \tag{7}$$

where $\boldsymbol{m} = (e/2m)\boldsymbol{r}\times\boldsymbol{p}$ is the magnetic dipole moment. The diamagnetic interaction is

$$\frac{e^2}{2m}A^2 = -\frac{e^2}{8m}(\boldsymbol{rr}-r^2\mathbf{1}):\boldsymbol{B}_0\boldsymbol{B}_0+\ldots. \tag{8}$$

Thus (1) can be written directly in multipole form when the fields are static.

3. Dynamic fields

If the fields are dynamic, $\boldsymbol{B}$ is still determined by $\boldsymbol{A}$ alone, whereas $\boldsymbol{E}$ is determined by both $\boldsymbol{A}$ and ϕ:

$$\boldsymbol{E}(\boldsymbol{r},t) = -\nabla\phi(\boldsymbol{r},t)-\dot{\boldsymbol{A}}(\boldsymbol{r},t) \tag{9}$$

$$\boldsymbol{B}(\boldsymbol{r},t) = \nabla\times\boldsymbol{A}(\boldsymbol{r},t). \tag{10}$$

There is gauge freedom in the choice of ϕ and A. We make an explicit choice with the Taylor series representations

$$\phi(r, t) = -r \cdot E_0(t) - \tfrac{1}{2} rr : (\nabla E(t))_0 + \dots \tag{11}$$

$$A(r, t) = \tfrac{1}{2} B_0(t) \times r + \tfrac{1}{3} r \cdot (\nabla B(t))_0 \times r + \dots, \tag{12}$$

which satisfy (9) and (10) if E and B can be Taylor expanded:

$$E(r, t) = E_0(t) + r \cdot (\nabla E(t))_0 + \dots \tag{13}$$

$$B(r, t) = B_0(t) + r \cdot (\nabla B(t))_0 + \dots. \tag{14}$$

(For simplicity we have not included ϕ_0 in (11); this can be added at the end if required, but in any case the corresponding energy will vanish if a neutral collection of charges is considered.) It is easy to verify that (11) and (12) lead to (13) and (14). The constant terms E_0 and B_0 are obvious. To see how the term $r \cdot (\nabla E(t))_0$ in (13) arises, we use the relations

$$\tfrac{1}{2} \nabla \{ rr : (\nabla E(t))_0 \} = r \cdot (\nabla E(t))_0^{\mathrm{S}} \tag{15}$$

$$\frac{1}{2} \frac{\partial}{\partial t} (B_0(t) \times r) = \frac{1}{2} (-\nabla \times E(t))_0 \times r = r \cdot (\nabla E(t))_0^{\mathrm{A}} \tag{16}$$

where T^{S} and T^{A} denote the symmetric and antisymmetric parts of a tensor $T = T^{\mathrm{S}} + T^{\mathrm{A}}$ and use has been made of the Maxwell equation $\nabla \times E = -\dot{B}$. Substituting (11) and (12) in (1) leads to the dynamic multipole interaction Hamiltonian

$$V(t) = -\boldsymbol{\mu} \cdot E_0(t) - Q : (\nabla E(t))_0 - m \cdot B_0(t) + \dots \tag{17}$$

plus the dynamic diamagnetic terms

$$-\frac{e^2}{8m} (rr - r^2 \mathbf{1}) : B_0(t) B_0(t) + \dots. \tag{18}$$

Notice that the gauge implied by the choice (11) and (12) does not correspond to the Coulomb gauge ($\nabla \cdot A = 0$) or the Lorentz gauge ($\nabla \cdot A = -\dot{\phi}$).

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