INTERNATIONAL SERIES OF MONOGRAPHS ON PHYSICS • 128

Multipole Theory in Electromagnetism

Classical, Quantum, and Symmetry Aspects, with Applications

R. E. RAAB
O. L. DE LANGE

OXFORD SCIENCE PUBLICATIONS

THE
INTERNATIONAL SERIES
OF
MONOGRAPHS ON PHYSICS

International Series of Monographs on Physics

128. R. E. Raab, O. L. de Lange: *Multipole theory in electromagnetism*
127. A. Larkin, A. Varlamov: *Theory of fluctuations in superconductors*
126. P. Goldbart, N. Goldenfeld, D. Sherrington: *Stealing the gold*
125. S. Atzeni, J. Meyer-ter-Vehn: *The physics of inertial fusion*
124. C. Kiefer: *Quantum Gravity*
123. T. Fujimoto: *Plasma Spectroscopy*
122. K. Fujikawa, H. Suzuki: *Path integrals and quantum anomalies*
121. T. Giamarchi: *Quantum physics in one dimension*
120. M. Warner, E. Terentjev: *Liquid crystal elastomers*
119. L. Jacak, P. Sitko, K. Wieczorek, A. Wójs: *Quantum Hall systems*
118. J. Wesson: *Tokamaks Third edition*
117. G. Volovik: *The universe in a helium droplet*
116. L. Pitaevskii, S. Stringari: *Bose–Einstein condensation*
115. G. Dissertori, I. G. Knowles, M. Schmelling: *Quantum chromodynamics*
114. B. DeWitt: *The global approach to quantum field theory*
113. J. Zinn-Justin: *Quantum field theory and critical phenomena, Fourth edition*
112. R. M. Mazo: *Brownian motion—fluctuations, dynamics, and applications*
111. H. Nishimori: *Statistical physics of spin glasses and information processing—an introduction*
110. N. B. Kopnin: *Theory of nonequilibrium superconductivity*
109. A. Aharoni: *Introduction to the theory of ferromagnetism, Second edition*
108. R. Dobbs: *Helium three*
107. R. Wigmans: *Calorimetry*
106. J. Kübler: *Theory of itinerant electron magnetism*
105. Y. Kuramoto, Y. Kitaoka: *Dynamics of heavy electrons*
104. D. Bardin, G. Passarino: *The Standard Model in the making*
103. G. C. Branco, L. Lavoura, J. P. Silva: *CP violation*
102. T. C. Choy: *Effective medium theory*
101. H. Araki: *Mathematical theory of quantum fields*
100. L. M. Pismen: *Vortices in nonlinear fields*
99. L. Mestel: *Stellar magnetism*
98. K. H. Bennemann: *Nonlinear optics in metals*
97. D. Salzmann: *Atomic physics in hot plamas*
96. M. Brambilla: *Kinetic theory of plasma waves*
95. M. Wakatani: *Stellarator and heliotron devices*
94. S. Chikazumi: *Physics of ferromagnetism*
91. R. A. Bertlmann: *Anomalies in quantum field theory*
90. P. K. Gosh: *Ion traps*
89. E. Simánek: *Inhomogeneous superconductors*
88. S. L. Adler: *Quaternionic quantum mechanics and quantum fields*
87. P. S. Joshi: *Global aspects in gravitation and cosmology*
86. E. R. Pike, S. Sarkar: *The quantum theory of radiation*
84. V. Z. Kresin, H. Morawitz, S. A. Wolf: *Mechanisms of conventional and high* T_c *superconductivity*
83. P. G. de Gennes, J. Prost: *The physics of liquid crystals*
82. B. H. Bransden, M. R. C. McDowell: *Charge exchange and the theory of ion-atom-collision*
81. J. Jensen, A. R. Mackintosh: *Rare earth magnetism*
80. R. Gastmans, T. T. Wu: *The ubiquitous photon*
79. P. Luchini, H. Motz: *Undulators and free-electron lasers*
78. P. Weinberger: *Electron scattering theory*
76. H. Aoki, H. Kamimura: *The physics of interacting electrons in disordered systems*
75. J. D. Lawson: *The physics of charged particle beams*
73. M. Doi, S. F. Edwards: *The theory of polymer dynamics*
71. E. L. Wolf: *Principles of electron tunneling spectroscopy*
70. H. K. Henisch: *Semiconductor contacts*
69. S. Chandrasekhar: *The mathematical theory of black holes*
68. G. R. Satchler: *Direct nuclear reactions*
51. C. Møller: *The theory of relativity*
46. H. E. Stanley: *Introduction to phase transitions and critical phenomena*
32. A. Abragam: *Principles of nuclear magnetism*
27. P. A. M. Dirac: *Principles of quantum mechanics*
23. R. E. Peierls: *Quantum theory of solids*

Multipole Theory in Electromagnetism

Classical, quantum, and symmetry aspects, with applications

R. E. RAAB
O. L. DE LANGE

School of Chemical and Physical Sciences, University of Natal, Pietermaritzburg, South Africa

CLARENDON PRESS · OXFORD
2005

OXFORD
UNIVERSITY PRESS
Great Clarendon Street, Oxford OX2 6DP
Oxford University Press is a department of the University of Oxford.
It furthers the University's objective of excellence in research, scholarship,
and education by publishing worldwide in
Oxford New York
Auckland Bangkok Buenos Aires Cape Town Chennai
Dar es Salaam Delhi Hong Kong Istanbul
Karachi Kolkata Kuala Lumpur Madrid Melbourne Mexico City Mumbai
Nairobi São Paulo Shanghai Taipei Tokyo Toronto
Oxford is a registered trade mark of Oxford University Press
in the UK and in certain other countries
Published in the United States
by Oxford University Press Inc., New York

First published 2005

A catalogue record for this title is available from the British Library
Library of Congress Cataloging in Publication Data
(Data available)
ISBN 0 19 856727 8
10 9 8 7 6 5 4 3 2 1
Printed in Great Britain
on acid-free paper by
Biddles Ltd, Kings Lynn, Norfolk

PREFACE

It is a capital mistake to theorize before one has data.
Arthur Conan Doyle
(*Scandal in Bohemia*)

Multipole expansions in electrostatics, magnetostatics, and electrodynamics provide a useful and powerful method of characterizing charge and current distributions, and the associated electromagnetic potentials and fields. When applied to macroscopic electrodynamics, and used in conjunction with quantum mechanics and relevant space–time properties and symmetries of physical quantities, multipole theory enables one to describe certain macroscopic electromagnetic phenomena in terms of the underlying microscopic structure — molecules for gases and unit cells for crystals. For example, one can relate birefringences (natural and induced), dichroisms, and reflectivities to polarizabilities and multipole moments of the microscopic unit. Where phenomena require that both electric and magnetic contributions be considered, as in certain transmission effects in crystals, multipole theory provides a way of circumventing the otherwise intractable nature of the problem (Section 5.13).

Although there are several excellent books on electromagnetic theory, none concentrates exclusively on multipole theory; this despite the considerable research that has been reported on applications, and even the formulation, of multipole theory during the last few decades. This circumstance provides the motivation for the present book.

It might be thought that the formulation and applications of multipole theory in macroscopic electromagnetism are, in principle, straightforward and lacking in surprises or undue subtlety. The first indication to the contrary occurs in linear constitutive relations for the electromagnetic response fields **D** and **H** obtained directly from multipole theory. The dynamic material constants (permittivity, permeability, and magnetoelectic coefficients) in these relations have the surprising and unphysical feature that, for contributions beyond electric dipole order, they are not translationally invariant (independent of the choice of origin of coordinates). A further surprise follows: despite this defect, one can use multipole theory to construct a satisfactory theory of transmission effects. This happy circumstance does not extend to reflection effects, for which existing multipole theory yields fundamentally unphysical results when taken beyond electric dipole order, notably reflected intensities that are not translationally invariant.

These difficulties arise in the following way. Multipole theory expresses observables in terms of quantities which are, in general, origin dependent: namely, polarizabilities (and sometimes also multipole moments). Therefore, in the description of origin-independent observables, the theory should combine various polarizabilities (and multipole moments) in such a manner that the overall expression is origin independent. It does this successfully for transmission and scattering phenomena (Chapter 5), but not for the dynamic material constants (Chapter 4) or reflection phenomena (Chapter 6). Thus multipole theory in macroscopic electromagnetism presents a rather puzzling picture.

Our purpose in writing this monograph has been three-fold. First, we intend it as a detailed introduction to classical, quantum-mechanical, and symmetry aspects of multipole theory in electromagnetism. We consider both a charge distribution in vacuum and, by extension, bulk matter (Chapters 1 to 3). This extension involves an averaging technique which yields the macroscopic multipole moment densities; we do not discuss the details of this technique because there are comprehensive treatments in the literature.

Second, we provide an account of some of the successes and failures of the direct application of multipole theory to macroscopic media. This is presented in Chapters 4 to 6 which deal with constitutive relations and transmission, scattering, and reflection phenomena. These chapters should be of interest and value to the novice and experienced researcher alike, since the existing extensive literature is rather fragmented, sometimes misleading, and occasionally incomplete, making it difficult to assess the state of this subject. For instance, one will search the literature in vain for any demonstration, such as that of Section 6.8, of the unphysical nature of the multipole theory of reflection from crystal surfaces. In our selection of topics for inclusion in Chapters 4 to 6 we have omitted certain standard applications of multipole theory, such as those in electrostatics and magnetostatics, because these are available in several texts on electromagnetism.

Our third purpose in writing this monograph is to present an alternative to the unphysical standard formulation of multipole theory for macroscopic media. We exploit the non-uniqueness of the response fields **D** and **H** in Maxwell's macroscopic equations to construct a transformation theory for these fields (Chapter 7). This transformation theory is designed to restore the translational invariance of the theory, thereby changing unphysical multipole constitutive relations into unique, physically acceptable relations. It also modifies expressions for macroscopic multipole moment densities in a desirable manner and restores the Post constraint for the magnetoelectric tensors (Chapter 8). In Chapter 9 we show that this transformation theory retains the good features of the standard formulation of multipole theory, as exemplified by its application to transmission phenomena, while it removes the undesirable features of this theory, such as its unphysical consequences for reflection phenomena.

The required background for reading this monograph is a knowledge of introductory electromagnetic theory (including Maxwell's equations in vacuum), and introductory non-relativistic quantum mechanics (in the Dirac formalism and including perturbation theory). A reader who is already acquainted with multipole theory, and who is interested in the unphysical aspects of this theory and their resolution, may commence reading at Chapter 4. To assist the reader, a glossary of symbols is provided at the end of the book.

The content of this book, in part or in whole, should appeal to a broad spectrum of scientists: to physics students wishing to advance their knowledge of multipole theory beyond the treatment offered in texts on electromagnetism; to optical and molecular physicists, researchers in ellipsometry, physical and theoretical chemists who conduct research related to multipole effects; to solid state physicists studying the effects of static and dynamic fields in condensed matter; to engineers with interests ranging from microwave effects in synthetic chiral and other materials to free-space radiation; and to applied mathematicians developing theories of anisotropic materials.

The advent of increasingly powerful computers and computational techniques has brought a most interesting development. Recent *ab initio* numerical calculations by several researchers have shown that the accurate evaluation of rather complicated polarizabilities and hyperpolarizabilities is now feasible. These studies provide strong support for the multipole approach (Sections 5.11 and 5.12). It is likely that the combination of experiment, theory, and computational research will lead to further progress in the understanding of complex electromagnetic systems. We therefore hope that our book will stimulate interest in this topic among students of physics, chemistry, and mathematics, and that it will assist computational physicists and chemists wishing to work in this area to acquire the necessary background in multipole theory.

Each field of endeavour has a beginning, even if serendipitous. For one of us (RER) there were the immediate inspiration and solid foundation provided by Professor David Buckingham, CBE, FRS, to his first research student in the field of multipoles and their applications. David's ongoing interest in the molecular physics group at the University of Natal[1] has been a source of much encouragement. Some of the material in this book draws on the collaborative research undertaken over many years with Dr. Elizabeth Graham and Professor Clive Graham and a succession of excellent research students. Their contributions are gratefully acknowledged.

Pietermaritzburg, South Africa R. E. R.
May 2004 O. L. de L.

[1]The University of Natal merged with the University of Durban-Westville on 1 January 2004 to become the University of KwaZulu-Natal.

This page intentionally left blank

CONTENTS

1

CLASSICAL MULTIPOLE THEORY

And mighty folios first, a lordly band,
Then quartos, their well-order'd ranks maintain,
And light octavos fill a spacious plain;
See yonder, ranged in more frequent rows,
A humbler band of duodecimos.
George Crabbe
(*The library*)

In this chapter we present an introduction to classical multipole theory. This is first discussed for electrostatics (Sections 1.1–1.5) and magnetostatics (Sections 1.6–1.9). Multipole expansions of the scalar and vector potentials for time-dependent charge and current distributions are derived (Section 1.10), together with their far- and near-zone limits (Section 1.11). Macroscopic media are considered in Section 1.12, where the macroscopic multipole moment densities are introduced, and it is shown how bound charge and current densities can be expressed in terms of these multipole moment densities. This leads to a discussion of Maxwell's macroscopic equations and expressions for the response fields **D** and **H** in terms of multipole moment densities (Section 1.13). The use of primitive versus traceless moments is discussed in Section 1.15.

Multipole expansions are represented by infinite series such as (1.3), (1.47), (1.76), (1.78), (1.118), and (1.119). In this book, the highest multipole order to which we present explicit results is electric octopole–magnetic quadrupole. There are two reasons for this. First, this is the highest order to which physical effects have been studied (Section 2.12 and Chapter 5). Second, working to this order is useful in elucidating aspects of the theory (Chapter 4).

1.1 Multipole expansion for the potential of a finite static charge distribution

We consider a finite, continuous distribution of charge in vacuum, and choose an origin of coordinates O inside the distribution. The charge inside an infinitesimal volume element dv is $\rho(\mathbf{r})\,dv$ where ρ is the charge density and $\mathbf{r}$ is the position vector of dv (see Fig. 1.1). Let P be a field point with position vector $\mathbf{R}$. The electrostatic potential at P is

$$\Phi(\mathbf{R}) = \frac{1}{4\pi\varepsilon_0}\int_V \frac{\rho(\mathbf{r})\,dv}{|\mathbf{R}-\mathbf{r}|}\,, \tag{1.1}$$

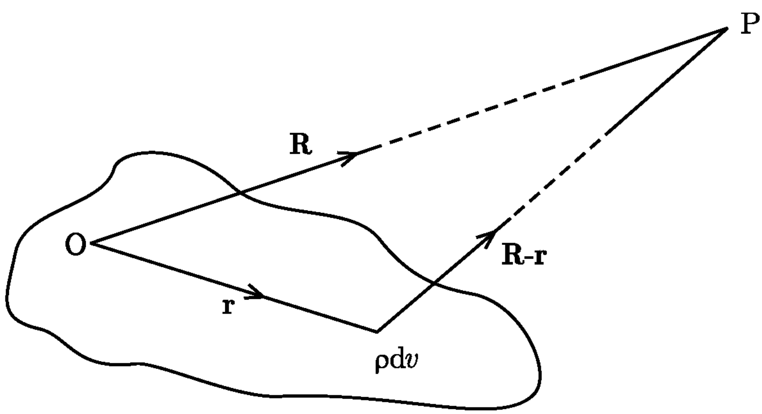

FIG. 1.1. Coordinates and notation for a finite, continuous charge distribution.

where, for a distribution of volume V, we have taken the zero of potential at infinity. Next, we consider a distant field point ($R \gg r$) and expand

$$\begin{aligned}
|\mathbf{R}-\mathbf{r}|^{-1} &= (R^2 - 2\mathbf{R}\cdot\mathbf{r} + r^2)^{-1/2} \\
&= \frac{1}{R}\left(1 + \frac{1}{R^2}\left[r^2 - 2\mathbf{R}\cdot\mathbf{r}\right]\right)^{-1/2} \\
&= \frac{1}{R} + \frac{\mathbf{R}\cdot\mathbf{r}}{R^3} + \frac{3(\mathbf{R}\cdot\mathbf{r})^2 - R^2 r^2}{2R^5} + \frac{5(\mathbf{R}\cdot\mathbf{r})^3 - 3R^2(\mathbf{R}\cdot\mathbf{r})r^2}{2R^7} + \cdots,
\end{aligned} \tag{1.2}$$

where in the last step we have used the binomial expansion and grouped terms in powers of **r**.

From (1.1) and (1.2) we obtain the multipole expansion for the electrostatic potential at P relative to the origin O

$$\begin{aligned}
\Phi(\mathbf{R}) = \frac{1}{4\pi\varepsilon_0}\Bigg[&\frac{q}{R} + \frac{R_i}{R^3}p_i + \frac{3R_iR_j - R^2\delta_{ij}}{2R^5}q_{ij} \\
&+ \frac{5R_iR_jR_k - R^2(R_i\delta_{jk} + R_j\delta_{ki} + R_k\delta_{ij})}{2R^7}q_{ijk} + \cdots\Bigg].
\end{aligned} \tag{1.3}$$

Here δ_{ij} is the Kronecker delta function ($\delta_{ij} = 1$ if $i = j$, $\delta_{ij} = 0$ if $i \neq j$) and q, p_i, q_{ij}, $q_{ijk}, \ldots$ are electric multipole moments, relative to the origin O, defined as follows:

$$q = \int_V \rho(\mathbf{r})\,dv \tag{1.4}$$

is the zeroth moment, or electric monopole moment,

$$p_i = \int_V r_i\,\rho(\mathbf{r})\,dv \tag{1.5}$$

is the first moment, or electric dipole moment,

$$q_{ij} = \int_V r_i r_j \, \rho(\mathbf{r}) \, dv \tag{1.6}$$

is the second moment, or electric quadrupole moment,

$$q_{ijk} = \int_V r_i r_j r_k \rho(\mathbf{r}) \, dv \tag{1.7}$$

is the third moment, or electric octopole moment, and so on. In (1.3) we have introduced a notation which will be used throughout this book: a subscript $i, j, \ldots$ (= 1, 2, or 3) denotes a component of a Cartesian tensor, and a repeated subscript implies summation from 1 to 3. In (1.3) we have written the expansion explicitly to electric octopole order. (A reader who is unfamiliar with Cartesian tensors may find it helpful to refer to Section 3.3.)

For a finite, discrete charge distribution with N charges $q^{(\alpha)}$ $(\alpha = 1, 2, \ldots, N)$ located at positions $\mathbf{r}^{(\alpha)}$ one starts with

$$\Phi(\mathbf{R}) = \frac{1}{4\pi\varepsilon_0} \sum_{\alpha=1}^{N} \frac{q^{(\alpha)}}{|\mathbf{R} - \mathbf{r}^{(\alpha)}|}, \tag{1.8}$$

instead of (1.1). (Here we have, for clarity of notation, used a superscript α to label the charges: an alternative notation which is frequently used in the literature assigns two subscripts to a vector—one labelling the particle, the other its Cartesian component [1, 2].) The result is the expansion (1.3) with

$$q = \sum_{\alpha=1}^{N} q^{(\alpha)} \tag{1.9}$$

$$p_i = \sum_{\alpha=1}^{N} q^{(\alpha)} r_i^{(\alpha)} \tag{1.10}$$

$$q_{ij} = \sum_{\alpha=1}^{N} q^{(\alpha)} r_i^{(\alpha)} r_j^{(\alpha)} \tag{1.11}$$

$$q_{ijk} = \sum_{\alpha=1}^{N} q^{(\alpha)} r_i^{(\alpha)} r_j^{(\alpha)} r_k^{(\alpha)} \tag{1.12}$$

for the first four electric multipole moments. An alternative method of deducing (1.9)–(1.12) uses the Dirac delta function: this function is defined by $\delta(\mathbf{r}) = 0$ if $\mathbf{r} \neq 0$ and

$$\int \delta(\mathbf{r}) \, dv = 1$$

if the region of integration includes the origin. If we replace $\rho(\mathbf{r})$ in (1.4)–(1.7) with $\sum_{\alpha=1}^{N} q^{(\alpha)} \delta(\mathbf{r} - \mathbf{r}^{(\alpha)})$ for a discrete distribution, we obtain (1.9)–(1.12).

The electric field $\mathbf{E} = -\boldsymbol{\nabla}\Phi$ can be found from (1.3). Writing $E_i = -\partial\Phi/\partial R_i$ we obtain

$$E_i(\mathbf{R}) = \frac{1}{4\pi\varepsilon_0}\left[\frac{R_i}{R^3}q + \frac{3R_iR_j - R^2\delta_{ij}}{R^5}p_j + \frac{3}{2R^7}\left\{5R_iR_jR_k - R^2(R_i\delta_{jk} + R_j\delta_{ki} + R_k\delta_{ij})\right\}q_{jk} + \cdots\right]. \quad (1.13)$$

The expansions (1.3) and (1.13) show that:

(i) Each multipole contributes separately to the potential and field at an external point.

(ii) Each multipole behaves as if it were located at the origin. This is because its contribution to the potential and field contains, apart from the moment itself, only $\mathbf{R}$, the displacement of the field point P from the origin O.

(iii) The potential and field due to each multipole depend not only on its moment and on its distance R from the field point, but in general also on its orientation relative to $\mathbf{R}$. For example, the dipole contribution in (1.3) and (1.13) contains $R_ip_i = Rp\cos\theta$, where θ is the angle between $\mathbf{R}$ and $\mathbf{p}$.

(iv) The R-dependences of the potential and field, respectively, are charge: R^{-1} and R^{-2}; dipole: R^{-2} and R^{-3}; quadrupole: R^{-3} and R^{-4}, etc.

(v) At sufficiently large distances (distance $\gg$ dimensions of charge distribution), the potential and field are dominated by the leading non-vanishing term in $1/R$, all higher-order terms being negligible. Associated with the leading non-vanishing term is a unique multipole moment independent of choice of origin (see Section 1.2). Thus, at a distant point the $SO_4^{=}$ ion behaves like a charge, HCl like a dipole, CO_2 like a quadrupole, CH_4 like an octopole, etc., even though each has higher moments. If the distance to the field point is not sufficiently large, then higher-order moments contribute as well.

(vi) The potential and field external to a neutral spherically symmetric charge distribution are zero.

We will refer to (1.4)–(1.7) and (1.9)–(1.12) as primitive moments to distinguish them from traceless moments which can be constructed for all terms beyond the electric dipole. For example, a commonly used definition of a traceless electric quadrupole moment is [1, 2]

$$\Theta_{ij} = \frac{1}{2}(3q_{ij} - q_{kk}\delta_{ij}). \quad (1.14)$$

Since $\delta_{ii} = 3$ we see that $\Theta_{ii} = 0$ as desired. According to (1.14), the quadrupole contribution to the potential (1.3) can be written as

$$\frac{1}{4\pi\varepsilon_0}\frac{3R_iR_j - R^2\delta_{ij}}{2R^5}\,\frac{1}{3}\left(2\Theta_{ij} + q_{kk}\delta_{ij}\right) = \frac{1}{4\pi\varepsilon_0}\frac{3R_iR_j - R^2\delta_{ij}}{3R^5}\Theta_{ij}.$$

Thus the term involving the trace q_{kk} in (1.14) does not contribute to the potential, and one can use either the primitive moment q_{ij} or the traceless moment Θ_{ij}

to calculate the quadrupole contribution to the potential, and hence the electric field. Now q_{ij} is symmetric and in general possesses six independent components, whereas the traceless property of Θ_{ij} means that it possesses five independent components. This reduction in the number of components is a consequence of Laplace's equation [3].

Higher-order traceless moments can be constructed in a similar manner, for example the traceless electric octopole moment [1, 4]

$$\Omega_{ijk} = \frac{1}{2}(5q_{ijk} - q_{ill}\delta_{jk} - q_{jll}\delta_{ki} - q_{kll}\delta_{ij}). \tag{1.15}$$

Again, the traces of the primitive moment q_{ijk} in (1.15) do not contribute to the potential (1.3), and one can use the traceless moment (1.15) to evaluate the octopole contribution to the potential.

The above definitions of traceless multipole moments are those used in molecular and crystal physics. Alternative definitions occur in the literature, such as [5] $\Theta_{ij} = q_{ij} - \frac{1}{3}q_{kk}\delta_{ij}$: with this definition the electrostatic potential (1.3) and field (1.13) are invariant under the replacement $q_{ij} \to \Theta_{ij}$. This property applies to electric multipoles of arbitrary order, and is indicative of the fact that for a pole of order 2^ℓ ($\ell = 0, 1, 2, \ldots$) in electrostatics, the electric multipole moment can be represented by a symmetric, traceless tensor of rank ℓ having $2\ell + 1$ independent components rather than the $\frac{1}{2}(\ell + 1)(\ell + 2)$ independent components of the corresponding primitive moment [5]. Thus in electrostatics, primitive moments beyond the dipole provide more components than are necessary. A similar property applies in magnetostatics (Section 1.6).

A convenient formulation of the theory of traceless multipole moments can be given in terms of spherical harmonics. We do not discuss this formulation here for two reasons. First, detailed accounts abound in the literature [3], [5–7]. Second, for the material presented in this monograph, it is more convenient to work in a Cartesian basis. For example, the Cartesian basis is more suitable for the derivation of macroscopic electrodynamics in multipole theory (Sections 1.10–1.13); for use in quantum theory of multipole moments and polarizabilities (Chapter 2); and to determine the origin dependence of polarizability tensors (Section 3.7). Use of this basis is also favoured in tables of space–time symmetries of property tensors (Section 3.6).

We will return to the topic of primitive and traceless multipole moments again in Section 1.15, particularly in relation to their role in macroscopic electromagnetism.

1.2 Dependence of electric multipole moments on origin

In general, electric multipole moments beyond the monopole depend on the choice of origin. Consider, for example, an electric quadrupole moment and an origin $\bar{O}$ displaced by $\mathbf{d}$ from O. The position vector of an element of charge $\rho\, dv$ relative to $\bar{O}$ is $\bar{\mathbf{r}} = \mathbf{r} - \mathbf{d}$. Thus the quadrupole moment (1.6) relative to $\bar{O}$ is

$$
\begin{aligned}
\bar{q}_{ij} &= \int_V (r_i - d_i)(r_j - d_j)\rho\, dv \\
&= q_{ij} - p_j d_i - p_i d_j + q d_i d_j, \qquad (1.16)
\end{aligned}
$$

where q and p_i are the moments (1.4) and (1.5). (Equation (1.16) also holds for the quadrupole moment (1.11) of a discrete charge distribution.) Thus the quadrupole moment is independent of an arbitrary shift of origin only if the monopole and dipole moments q and p_i are zero. This may be generalized: only the leading non-vanishing electric multipole moment is independent of the choice of origin of coordinates. The matter of origin dependence of certain physical quantities plays an important role in this book (see Chapters 3–9). For discussion of the origin dependence of electric quadrupole moments in relation to an experiment to measure these moments, see Section 5.11.

1.3 Permanent and induced multipole moments

The permanent multipole moments possessed by the static charge distribution $\rho(\mathbf{r})$ considered so far are denoted by

$$
p_i^{(0)}, \quad q_{ij}^{(0)}, \quad q_{ijk}^{(0)}, \quad \ldots, \qquad (1.17)
$$

to distinguish them from the multipole moments in the presence of an applied electric field. Consider first a uniform applied electric field. The charges in the distribution will be displaced to new equilibrium positions different from their field-free positions. The corresponding multipole moments (the total moments) are denoted by

$$
p_i, \quad q_{ij}, \quad q_{ijk}, \quad \ldots . \qquad (1.18)
$$

The differences

$$
p_i - p_i^{(0)}, \quad q_{ij} - q_{ij}^{(0)}, \quad q_{ijk} - q_{ijk}^{(0)}, \quad \ldots \qquad (1.19)
$$

are termed the induced electric multipole moments—dipole, quadrupole, octopole, ...

For a weak applied field one may assume that a given induced moment is proportional to the field. Then, for an anisotropic charge distribution,

$$
p_i - p_i^{(0)} = \alpha_{ij} E_j \qquad (1.20)
$$

$$
q_{ij} - q_{ij}^{(0)} = \mathfrak{a}_{ijk} E_k \qquad (1.21)
$$

$$
q_{ijk} - q_{ijk}^{(0)} = \mathfrak{b}_{ijkl} E_l, \text{ etc.} \qquad (1.22)
$$

In these α_{ij}, known as the (dipole) polarizability, is a constant of proportionality between the ith component of the induced dipole moment and the jth component of the uniform field that induces the moment. A similar role is played by $\mathfrak{a}_{ijk}$, termed the quadrupole polarizability (or quadrupolarizability), and $\mathfrak{b}_{ijkl}$, the octopole polarizability.

For a strong uniform field p_i may be expanded in powers of the field

$$p_i = p_i^{(0)} + \alpha_{ij} E_j + \frac{1}{2}\beta_{ijk} E_j E_k + \frac{1}{6}\gamma_{ijkl} E_j E_k E_l + \cdots . \tag{1.23}$$

This was used by Buckingham and Pople [8] in a theory of the Kerr effect, in which β_{ijk}, γ_{ijkl}, ... were collectively termed hyperpolarizabilities [9]. Like α_{ij} they are independent of the field and are thus properties of the unperturbed charge distribution. Similar expansions may be made for q_{ij}, q_{ijk}, ... At this stage equations (1.20)–(1.23) have only a phenomenological basis but they may be formally derived by means of quantum-mechanical time-independent perturbation theory (see Chapter 2). In much of this book only a linear response to a field, as in (1.20)–(1.22), will be assumed. An exception is the theory of the Kerr effect in Chapter 5.

A non-uniform electrostatic field also distorts a charge distribution, thereby inducing multipole moments. To electric octopole order the total moments may be expressed as (see Section 2.2)

$$p_i = p_i^{(0)} + \alpha_{ij} E_j + \frac{1}{2} a_{ijk} \nabla_k E_j + \frac{1}{6} b_{ijkl} \nabla_l \nabla_k E_j + \cdots \tag{1.24}$$

$$q_{ij} = q_{ij}^{(0)} + \mathfrak{a}_{ijk} E_k + \frac{1}{2} d_{ijkl} \nabla_l E_k + \cdots \tag{1.25}$$

$$q_{ijk} = q_{ijk}^{(0)} + \mathfrak{b}_{ijkl} E_l + \cdots . \tag{1.26}$$

The tensors $\mathfrak{a}_{ijk}$, $\mathfrak{b}_{ijkl}$, a_{ijk}, ... are also properties of the undistorted distribution. They are referred to collectively as polarizabilities. If a charge distribution is unaffected by an applied field, it is said to be non-polarizable or rigid.

In (1.24)–(1.26) it is assumed that the field is slowly varying inside the distribution; the field and its gradients are evaluated at the origin at which the point multipoles are located in the distribution. Again these expressions may be derived by means of quantum-mechanical perturbation theory, and this also yields explicit expressions for the polarizability tensors (Chapter 2), from which any intrinsic symmetry of tensor subscripts and relationships between certain tensors may be deduced. Thus (see Sections 2.2 and 2.7)

$$\begin{cases} \alpha_{ij} = \alpha_{ji}, \quad a_{ijk} = a_{ikj} = \mathfrak{a}_{jki} \\ b_{ijkl} = b_{ijlk} = b_{ikjl} = \mathfrak{b}_{jkli} \\ d_{ijkl} = d_{klij} = d_{jikl}. \end{cases} \tag{1.27}$$

1.4 Force and torque in an external electrostatic field

We consider a discrete charge distribution in an electrostatic field which is slowly varying. In the expression for the total force on the distribution

$$F_i = \sum_{\alpha=1}^{N} q^{(\alpha)} E_i(\mathbf{r}^{(\alpha)}) \tag{1.28}$$