Available online at www.sciencedirect.com
ScienceDirect
Annals of Physics 322 (2007) 799–823
ANNALS of PHYSICS
www.elsevier.com/locate/aop

Classical light dispersion theory in a regular lattice

M. Marino *, A. Carati, L. Galgani

Dipartimento di Matematica, Università di Milano, via Saldini 50, I-20133 Milano, Italy

Received 29 September 2005; accepted 22 November 2006
Available online 4 January 2007

Abstract

We study the dynamics of an infinite regular lattice of classical charged oscillators. Each individual oscillator is described as a point particle subject to a harmonic restoring potential, to the retarded electromagnetic field generated by all the other particles, and to the radiation reaction expressed according to the Lorentz–Dirac equation. Exact normal mode solutions, describing the propagation of plane electromagnetic waves through the lattice, are obtained for the complete linearized system of infinitely many oscillators. At variance with all the available results, our method is valid for any values of the frequency, or of the ratio between wavelength and lattice parameter. A remarkable feature is that the proper inclusion of radiation reaction in the dynamics of the individual oscillators does not give rise to any extinction coefficient for the global normal modes of the lattice. The dispersion relations resulting from our solution are numerically studied for the case of a simple cubic lattice. New predictions are obtained in this way about the behavior of the crystal at frequencies near the proper oscillation frequency of the dipoles.

PACS: 03.50.De; 41.20.Jb; 42.25.Lc; 78.20.Bh

---

1. Introduction

The classical theory of dispersion is a subject with a long and noble history [1,2]. Although the main features of the phenomenon can be described by treating matter as a continuum characterized by macroscopic quantities such as the electric and magnetic

---

[*] Corresponding author. Fax: +39 02 50316090.
E-mail addresses: Massimo.Marino@unimi.it (M. Marino), carati@mat.unimi.it (A. Carati), galgani@mat.unimi.it (L. Galgani).

0003-4916/$ - see front matter
doi:10.1016/j.aop.2006.11.006

polarizations, it is clear that a truly fundamental theory has to be based on a microscopic model of matter. We shall now try to summarize some crucial aspects of the problem in an historical perspective, before illustrating the new features of our present approach.

By treating an elementary electric dipole as an oscillator subject to a linear restoring force, it is possible to obtain a simple expression for the molecular polarizability, i.e., the complex frequency-dependent linear coefficient which relates the microscopic dipole moment to the amplitude of the incident electromagnetic radiation. In order to correctly apply this simple model to the description of the behavior of a large system of mutually interacting dipoles, one has however to consider that the field acting on each microscopic oscillator cannot be simply identified with the macroscopic electromagnetic field in the medium. In fact, while the latter simply represents the average of the microscopic field over a region much larger than the intermolecular spacing, the former has to be carefully calculated by evaluating and summing, on the site occupied by the considered dipole, the retarded fields generated by all the other dipoles of the medium. This "exciting" field (as we shall refer to in the following, although the names "effective" or "local" field have also been employed in the literature) was theoretically estimated by Lorentz already at the end of 19th century [3–6] by dividing the medium into two regions separated by a virtual sphere surrounding the considered dipole. He restricted his attention to the typical situation in which the wavelength of the macroscopic electromagnetic field is of a larger order of magnitude than the average intermolecular spacing, so that one can take for the virtual sphere a radius intermediate between the two. He then argued that the influence of the portion of the medium lying outside the sphere can be fairly approximated as that of a continuous distribution of electric dipole moment, whereas the sum of the forces exerted by all the dipoles situated inside the sphere can be assumed to vanish in most cases on the basis of symmetry considerations. A rather similar analysis, leading to equivalent conclusions, was also carried out by Planck [7]. With these arguments one can derive the well-known Lorentz–Lorenz formula [3,8], relating the macroscopic dielectric constant of the medium to the molecular polarizability, and it is thus possible to deduce an approximate expression for the dispersion relation of an array of oscillators in the long-wavelength regime (which generally includes the optical frequencies).

A detailed microscopic theory of dispersion in a crystalline solid, although with neglect of radiation reaction, was formulated by Ewald [9,10]. He considered a rectangular parallelepiped as the unit cell of the Bravais lattice, and his results were subsequently generalized by Born to more general crystal structures [1,11]. The mathematical methods used by these authors (one has to keep in mind that the theory of distributions was not yet existing at that time) led however to rather clumsy expressions for the exciting field, which could be numerically evaluated only in the limit of an infinitely large ratio between wavelength and lattice constant, i.e., still essentially in the continuum approximation. In this way the previous results by Lorentz and Planck were recovered for structures with tetrahedral symmetry. Furthermore, in the case of parallelepipeds of unequal edges, Ewald was able to perform in the same limit a numerical calculation relating the ratio between the edges to the phenomenon of double refraction. Finally, Ewald extended his analysis of the model also to the study of X-ray diffraction [12], but he made use to this purpose of other important simplifications which are possible only in the opposite limit of a radiation frequency much higher that the characteristic frequencies of the crystal.

Many investigations were later devoted to the application of quantum mechanics to the theory of light dispersion, and the results of Ewald and Born were apparently considered