

Mode Softening, Ferroelectric Transition, and Tunable Photonic Band Structures in a Point-Dipole Crystal

J. A. Klugkist, M. Mostovoy, and J. Knoester

*Institute for Theoretical Physics and Materials Science Center, University of Groningen,
Nijenborgh 4, 9747 AG Groningen, The Netherlands*

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We study the photonic band structure of cubic crystals of point dipoles. It is shown that in contrast to earlier claims these systems cannot have an omnidirectional photonic band gap. For sufficiently large plasma frequencies, however, they exhibit softening of photonic bands, leading to (anti)ferroelectric ordering of the dipoles and the possibility to open and tune directional band gaps by external electric fields. The model studied may be realized through lattices of quantum dots.

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The study of wave propagation through a periodic structure has had a long history, and still plays an important role in condensed matter physics. A conceptually simple example with a rich variety of physical properties is the propagation of electromagnetic waves through crystals of point dipoles. The oldest use of this model is the concept of the polariton and the polariton stop gap, describing the optical modes in atomic and molecular crystals [1,2]. More recently, crystals of point dipoles have also been used to model the propagation of light through photonic crystals. These are materials in which the refractive index is modulated with a period of the order of the wavelength of light. The multiple scattering in these crystals gives rise to the opening of photonic band gaps [3,4], in analogy to the electronic band gaps in semiconductors; photonic band gaps have been reproduced using lattices of point dipoles [5]. Photonic band gaps have interesting fundamental and technological consequences, such as the possibility to modify spontaneous emission [6], and the development of perfect mirrors and novel wave guides [7]. Other intriguing phenomena that have been predicted for point-dipole crystals are a negative refractive index and subwavelength lensing [8].

Recent advances in the fabrication of semiconductor and metallic quantum dots have opened new possibilities to realize materials that are well represented as crystals of point dipoles. The Mie or plasma resonances of the individual dots act as the dipolar transitions, with a wavelength much larger than the dot size [9]. It has been realized that arrays of closely spaced quantum dots, considered as point dipoles, may be used as subwavelength guides for electromagnetic energy (plasmonics) [10,11]. It has also been suggested that quantum dots forming two-dimensional lattices may spontaneously polarize as a consequence of the interdot dipolar interactions, even for lattice constants of the order of 100 nm [12].

Combining several of the above concepts, one may envision photonic crystals whose band structures soften as a consequence of electromagnetic interactions between

unit cells, leading to a dipole-ordered state at some critical interaction strength. Close to this instability, the band structure is expected to be very sensitive to external electric fields. This opens the possibility to tune photonic band gaps, a highly desired feature in photonics, for which several alternative methods have been suggested [13–18].

In this Letter, motivated by the above ideas, we perform a detailed study of the photonic band structure of cubic (sc, fcc, and bcc) point-dipole crystals. The dipole-light interaction couples the dipole excitations with a crystal wave vector \mathbf{k} to photons with wave vectors $\mathbf{k} + \mathbf{G}$, where \mathbf{G} is an arbitrary vector of the reciprocal lattice. This coupling, on the one hand, gives rise to the photonic bands and, on the other hand, results in long-range (retarded) interactions between the dipoles. We show that, in contrast to earlier claims [5], omnidirectional gaps do not occur in the band structure of these lattices. We also show that for sufficiently strong interactions the lowest photonic bands may soften at a particular symmetry point of the Brillouin zone, which leads to a dipole-ordered state, and we demonstrate the opening and tunability of directional band gaps when switching external electric fields close to the transition to this ordered state.

We consider a periodic array of transition dipoles, treated as harmonic oscillators with a frequency ω_0 , coupled linearly to the electromagnetic field. The Lagrangian reads (cf. Ref. [1])

$$L = \int dV \left[\frac{\mathbf{E}^2 - \mathbf{H}^2}{8\pi} + A^0 \nabla \cdot \mathbf{P} + \frac{\mathbf{A}}{c} \cdot \dot{\mathbf{P}} \right] + \frac{2\pi n}{\omega_p^2} \sum_j (\dot{\mathbf{p}}_j^2 - \omega_0^2 \mathbf{p}_j^2). \quad (1)$$

Here the plasmon frequency ω_p plays the role of a coupling constant, n is the density of dipoles and the polarization density is given by $\mathbf{P}(t, \mathbf{x}) = \sum_j \mathbf{p}_j(t) \delta(\mathbf{x} - \mathbf{R}_j)$, where \mathbf{R}_j are the coordinates of the lattice sites. Imposing the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ and eliminating A^0 , we obtain