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## Photonic Band Structure of Atomic Lattices

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A calculation of the optical band structure of a three dimensional lattice of resonant two-level atoms in the dipole approximation is presented. The formation of band gaps is exhibited and confirmed by a calculation of the density of states. The band structure can be characterized by two dimensionless parameters. We find a longitudinal polarization mode as well as a class of vacuum modes that are unaltered by the interaction with matter. Numerical calculations are performed for a face centered cubic lattice; other lattices can be evaluated as easily. [S0031-9007(96)01222-7]

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At present the study of *photonic crystals* [1], i.e., dielectric materials with a periodicity matching optical wavelengths, is a subject of active research. The periodicity induces an optical band structure quite analogous to the band structure in semiconductor physics. On both the theoretical (numerical) and experimental side, a search is going on for materials exhibiting a photonic *band gap*. Such a gap can give rise to the suppression of spontaneous emission of interstitial atoms and has promising consequences for applications. Moreover, from a fundamental point of view such materials, after some randomization, are interesting for the observation of the localization of light, and also the quantum electrodynamics of photonic crystals merits a further study [2]. Various authors have reported systems exhibiting photonic band gaps, depending on the type of unit cell, shape of the “atoms” [behavior of electric permeability  $\epsilon(\mathbf{x})$  over a unit cell], and refractive index contrast [1,3–5].

A similar band structure can arise in *atomic optical lattices*. Atoms, cooled down to the microkelvin regime, can be trapped in their ac Stark shift potential wells in a one, two, or three dimensional interference pattern created by a combination of laser beams. Consequently, the lattice constant is essentially the wavelength of the trapping field. Already results on Bragg scattering have been reported [6] showing long range periodic order. The main difference with the photonic crystals is the sharp resonant character of the scatterers (the atoms on the lattice sites) near an optical resonance in the atom. Furthermore, in the limit of weak light fields and if recoil effects are ignored, the propagation of light is coherent [7] and without dissipation. As a consequence, in a two-level approximation, atoms can be accurately described by classical damped linear point dipole oscillators possessing a sharp resonance. Here we calculate the band-structure properties of such a dipolar lattice. It leads to point interactions on the lattice sites which reduce the required computational effort immensely. Therefore our method is promising to be applied to more complicated lattices as well.

The starting point is the set of Maxwell’s equations for a static isotropic dielectric medium [permeability  $\epsilon(\omega, \mathbf{x}) \equiv 1 + 4\pi\chi(\omega, \mathbf{x})$ ] without external charges and currents. Elimination of the magnetic field component in favor of the electric field  $\mathbf{E}$  gives, after Fourier transformation with respect to time,

$$\partial_{\mathbf{x}} \times (\partial_{\mathbf{x}} \times \mathbf{E}) - 4\pi\chi(\omega, \mathbf{x})(\omega/c_0)^2 \mathbf{E} = (\omega/c_0)^2 \mathbf{E}, \quad (1)$$

where  $\chi(\omega, \mathbf{x})$  is the (linear) electric susceptibility and  $c_0$  the vacuum speed of light.

The atoms that build up the medium are modeled in the point dipole approximation. Since the atomic dimensions are small relative to the wavelength of optical fields, this makes good sense. The treatment of point dipoles within a scattering theory for electromagnetic waves was introduced by Wu [8]. Wu’s basic observation is that in setting the current  $\mathbf{J}(\mathbf{x}, t)$  in the Maxwell equation  $\partial_t \mathbf{E}(\mathbf{x}, t) = \partial_{\mathbf{x}} \times \mathbf{H}(\mathbf{x}, t) - \mathbf{J}(\mathbf{x}, t)$  proportional to  $\delta(\mathbf{x} - \mathbf{a})\mathbf{E}(\mathbf{x}, t)$ , where  $\mathbf{a}$  is the position of a point dipole, naturally leads to a point dipole interaction. In the present situation, where we have a polarization current  $\chi(\omega, \mathbf{x})(\omega/c_0)\mathbf{E}$ , due to the presence of an atom, a similar procedure can be followed:  $\chi(\omega, \mathbf{x}) \propto \delta(\mathbf{x} - \mathbf{a})\alpha(\omega)$  [9], where the resonance structure enters through  $\alpha(\omega)$ :

$$\alpha(\omega) = \frac{3c_0^3 \Delta}{\omega_0^2} \frac{1}{\omega_0^2 - \omega^2 - i2\Delta\omega^3/\omega_0^2}. \quad (2)$$

Equation (2) is the simplest classical representation of the typical linear polarizability (with linewidth parameter  $2\Delta$ ) for two-level atoms and damped oscillators [10]. Note that atoms characterized by (2) scatter light elastically: Its strength is fixed by the optical theorem [11].

We next turn to the lattice case where  $\chi(\omega, \mathbf{x})$  becomes periodic. We decompose  $\mathbf{E}$  in terms of the Bloch wave vectors  $\mathbf{k}$  in the first Brillouin zone and reciprocal lattice vectors  $\mathbf{g}$  as follows [12]:

$$\mathbf{E}_{\mathbf{k}}(\mathbf{x}) = \sum_{\mathbf{g}} \mathbf{E}(\mathbf{k} - \mathbf{g}) e^{i(\mathbf{k} - \mathbf{g}) \cdot \mathbf{x}}. \quad (3)$$

Next the susceptibility  $\chi$  is expanded in reciprocal lattice vectors  $\mathbf{g}$ :

$$\chi(\omega, \mathbf{x}) = \sum_{\mathbf{g}} \chi(\omega, \mathbf{g}) e^{i\mathbf{g}\cdot\mathbf{x}}. \quad (4)$$

Substitution of Eqs. (3) and (4) into Eq. (1) then results in

$$\left[ |\mathbf{k} - \mathbf{g}|^2 \Delta_{\mathbf{k}-\mathbf{g}} - \left( \frac{\omega}{c_0} \right)^2 \mathbf{I} \right] \cdot \mathbf{E}(\mathbf{k} - \mathbf{g}) - 4\pi \left( \frac{\omega}{c_0} \right)^2 \sum_{\mathbf{g}'} \chi(\omega, \mathbf{g}' - \mathbf{g}) \mathbf{E}(\mathbf{k} - \mathbf{g}') = 0, \quad (5)$$

where  $\mathbf{I}$  is the  $3 \times 3$  identity matrix and  $\Delta_{\mathbf{k}} = \mathbf{I} - \mathbf{e}_{\mathbf{k}} \mathbf{e}_{\mathbf{k}}$  ( $\mathbf{e}_{\mathbf{k}} \equiv \mathbf{k}/k$ ). Now Eq. (1) has been separated into a set of independent equations: one for each  $\mathbf{k}$  in the first Brillouin zone.

We are interested in the dispersion law  $\omega(\mathbf{k})$  from Eq. (5) for the dipolar lattice. It can be obtained by locating the poles of the  $t$  matrix for the whole lattice [13,14] and turns out to be implicit in the following  $3 \times 3$  determinantal condition:

$$\left\| \alpha(\omega)^{-1} \frac{c_0^2}{\omega^2} \mathbf{I} + \sum_{\mathbf{R}_i \neq \mathbf{0}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} \mathbf{G}_0(\omega, \mathbf{R}_i) \right\| = 0, \quad (6)$$

which in our numerical work has been implemented in reciprocal space. Here  $\mathbf{G}_0$  denotes the free-space Green's function for the Helmholtz equation (1) [8,13]. Diagonalization of the matrix in Eq. (6) physically represents summing over all light paths in the dipolar lattice. Its simplicity is due to the use of point interactions, their Fourier transform being independent of  $\mathbf{g}$ . For our model Eq. (6) coincides with the KKR condition used in band structure calculations in solid state physics [12,14].

We now turn to the results. We have solved  $\omega(\mathbf{k})$  numerically from Eq. (6) for a face centered cubic (fcc) lattice. We define two dimensionless parameters that characterize the band-structure picture completely. The first parameter is  $P \equiv (\omega_{\text{BZ}}/\omega_0)^3$ , which we will call here the "polariton parameter." We introduce  $\omega_{\text{BZ}}/c_0$  as the radius of the largest inscribing sphere of the Brillouin zone. It equals the modulus (in reciprocal space) of the  $L$  point, multiplied by  $c_0$ . Thus  $\omega_{\text{BZ}}/c_0 \equiv \pi\sqrt{3} \approx 5.44$ , where  $a$  is the lattice constant, and  $\omega_{\text{BZ}}$  relates to the density of scatterers as  $\rho \propto (\omega_{\text{BZ}}/c_0)^3$ . In terms of lengths we can say that  $P$  measures the ratio of the wavelength at resonance  $\lambda_0 \equiv 2\pi c_0/\omega_0$  and  $a$ . The second parameter is the quality factor  $Q \equiv \omega_0/2\Delta$  giving the sharpness of the resonance.

As an illustration we consider two characteristic choices for the combined parameter set  $(P, Q)$ . For parameter set 1 (Fig. 1), which represents the denser case,  $\omega_0$  is well below  $\omega_{\text{BZ}}$ :  $P = 1.29$  (corresponding with  $\lambda_0 = 1.26a$ ) and  $Q = 30$ . For parameter set 2 (Fig. 2):  $P = 0.47$  ( $\lambda_0 = 0.9a$ ) and  $Q = 21$ . In both Figs. 1 and 2 we still see the linear dispersion law around the origin  $\Gamma$  of the Brillouin zone. There is a

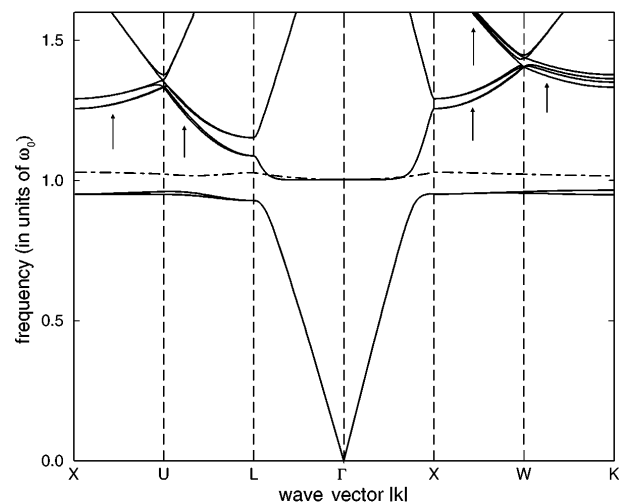


FIG. 1. Photonic band structure for a fcc lattice of resonant dipoles. The resonance wavelength  $\lambda_0$  for this case equals  $\lambda_0 = 1.26a$  ( $P = 1.29$  and  $Q = 30$  in Fig. 4). Horizontally, we have parametrized a path along the symmetry points  $X, U, L, \Gamma, X, W, K$  in the Brillouin zone. The dot-dashed line is a longitudinal polarization mode; the arrows indicate the vacuum modes that is unaltered by the interaction (see text).

polarization degeneracy (for all modes but one) that is frequently lifted. Only one mode, the relatively straight dot-dashed line in the middle of Fig. 1 and upper part of Fig. 2, is not degenerate. Moreover, inspection of its corresponding eigenfunction shows that it is mainly longitudinal (parallel to  $\mathbf{k}$ ). It can therefore be interpreted as a coupling of light with the *longitudinal* polarization field. It originates from the dispersion law associated with (2) which exhibits negative values of the dielectric function. A simple estimate for the approximate position of the line at  $\mathbf{k} = \mathbf{0}$  is given by the zero of the dielectric function  $\varepsilon(\omega_{\text{LO}}) = 1 + 4\pi\rho\alpha(\omega_{\text{LO}}) \equiv 0$ , from which

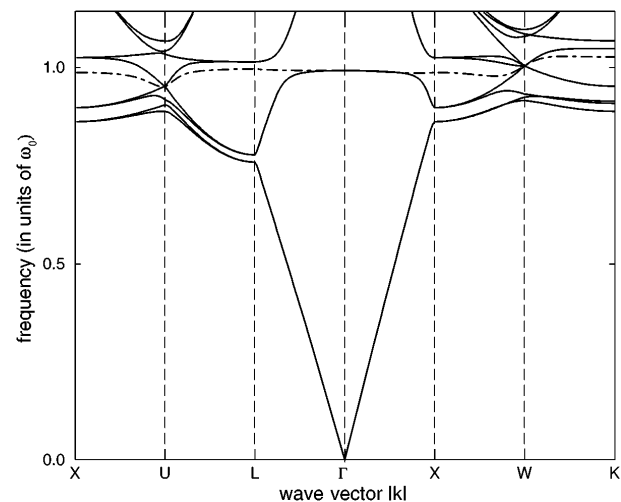


FIG. 2. As in Fig. 1, but now for the more dilute case that  $\lambda_0 = 0.9a$  ( $P = 0.47$  and  $Q = 21$  in Fig. 4).

follows  $\omega_{LO} = 5.05c_0/a$  [12]; from Fig. 1 we have  $\omega_{LO} = 5.02c_0/a$ . Also in Fig. 1 the two branches in the lowest band level off at the boundary of the Brillouin zone, where they stay below the resonance frequency. In this flat region the dispersion is material-like, which indicates a polariton type of propagation in the crystal [12].

At the points  $U, L, X$ , and  $W$  one observes the occurrence of avoided crossings; a phenomenon that in other physical situations may coincide with the presence of a Kronig-Penney type of band gap [1,3–5]. A genuine band gap, however, seems to exist only around the resonance frequency in Fig. 1. Whether or not a band gap exists can be ascertained by considering every value of  $\mathbf{k}$  in the Brillouin zone. This calls for a calculation of the density of states (DOS)  $N(\omega)$  [15]:

$$N(\omega) = 2\omega \sum_{n,\mathbf{k}} \delta(\omega^2 - \omega_n^2(\mathbf{k})). \quad (7)$$

Here  $n$  denotes a band index; all polarization modes have a separate band index. In Fig. 3  $N(\omega)$  has been plotted for both parameter sets, scaled by the vacuum DOS  $N_0(\omega)$ . In the neighborhood of the resonance frequency, we see the corresponding resonant enhancement of the DOS. We see from Fig. 3 that for set 1 a gap is indeed present, whereas for set 2 no gap is found, although a pronounced structure around the resonance frequency remains.

We have investigated the possible presence of a gap for given values of  $P$  and  $Q$ : The resulting “phase diagram” is depicted in Fig. 4. Apparently a gap exists *always* for  $P \geq 1.0$ , independently of  $Q$ . In terms of the resonant wavelength, this condition translates to  $\lambda_0 \geq 1.15a$ . The line  $P = 1.0$  constitutes for high values of  $Q$  an asymptotic boundary for the left region, where no gap is found. For smaller values of  $Q$ , say  $Q \lesssim 50$

(corresponding with a broad resonance), the lower bound on  $P$  decreases. Note, however, that for atoms  $Q \gg 50$ . For reasons of graphical representation we have chosen low values of  $Q$  since the width of the gap  $\Delta\omega \sim Q^{-1}$ . From Fig. 3 we observe that  $\Delta\omega/\omega_0 \approx 0.85Q^{-1}$ . The absence of a gap for  $\omega_0 > \omega_{BZ}$  can be clarified by considering the lines in Fig. 1 that are indicated by arrows. These lines are identically present for all values of  $P$  and  $Q$  and coincide with eigenvalues of the *empty lattice*. Thus free eigenvalues in some bands remain eigenvalues of the perturbed system (which is not true for the associated eigenfunctions). This feature was observed earlier in the Schrödinger case [16] (p. 189). There it is shown that  $\omega = c_0(\mathbf{k} - \mathbf{g})$  is an eigenvalue of multiplicity  $m \geq 1$  if, and only if, there are  $m + 1$  reciprocal lattice vectors  $\mathbf{g}_0, \mathbf{g}_1, \dots, \mathbf{g}_m$  such that

$$|\mathbf{k} - \mathbf{g}_0| = |\mathbf{k} - \mathbf{g}_1| = \dots = |\mathbf{k} - \mathbf{g}_m|. \quad (8)$$

This is precisely what we find in our numerical work, both for the scalar (see below) and Maxwell cases. Because of (8), this type of eigenvalue occurs only at  $\mathbf{k}$  values of a certain symmetry. The rigidity of these lines disturbs the formation of a band gap when  $\omega_0$  exceeds the minimum value  $\omega_{BZ}$ .

Usually for photonic crystals the frequency gaps are found near or above the boundary of the Brillouin zone [3–5] where the periodicity is nearly matched. Their formation is similar to that of the gaps found in the Kronig-Penney model. It has therefore been argued that the fcc lattice is favorable for finding an isotropic band gap. Its Brillouin zone coming closest to a sphere implies a maximum overlap for the gaps in all directions [3]. In contrast, our gap is a direct consequence of the nature of the resonant interaction. It is found *below* the boundary of the Brillouin zone; therefore the role of the geometry of the Brillouin zone (and corresponding Bravais lattice) may be viewed as less critical.

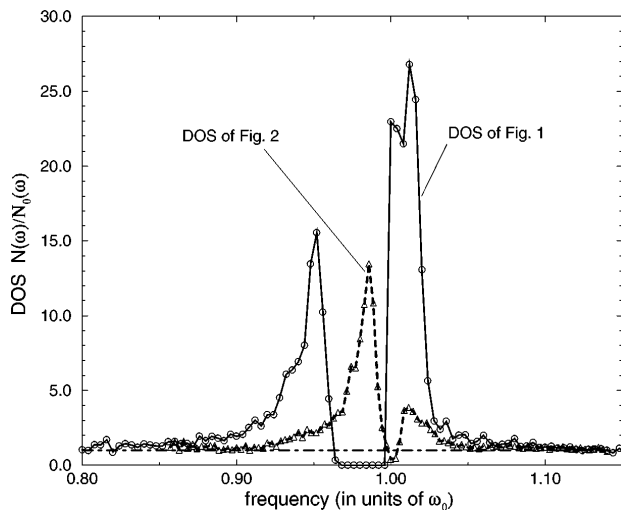


FIG. 3. Scaled density of states for the two special cases of Figs. 1 and 2.

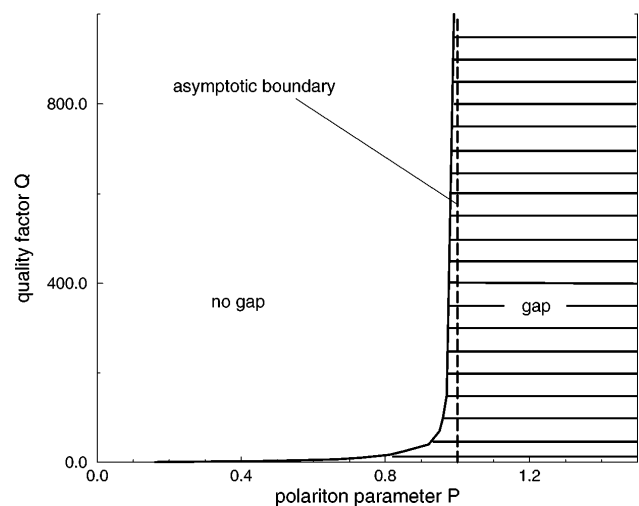


FIG. 4.  $P, Q$  “phase diagram.”

This statement is confirmed by the fact that the scalar wave approximation is excellent in our case. The Helmholtz equation (1) is frequently approximated by the scalar wave equation

$$-\partial_{\mathbf{x}}^2 \Psi - 4\pi \chi(\omega, \mathbf{x}) (\omega/c_0)^2 \Psi = (\omega/c_0)^2 \Psi, \quad (9)$$

which is known to be inadequate in general. There are cases where band gaps show up in the scalar wave approximation which are absent in a vector picture and vice versa 50 [1,3–5]. In our case, however, the difference in eigenvalues is uniformly less than 1%. The longitudinal mode is absent here as it should be for scalar waves.

In conclusion, we have solved the optical band structure and density of states for a lattice of resonant classical dipole oscillators. We infer that the band structure (and existence of a gap) is determined entirely by two dimensionless parameters, which measure the scattering strength and the width of the atomic resonance, respectively. For today's experimentally realizable optical lattices two remarks are in order. First, oscillatory motion of the atoms around the equilibrium position has been neglected in our model. In a more elaborate treatment this could be accounted for by means of the Debye-Waller (DW) factor [12], as was done in an observation of Bragg scattering from atomic lattices in Ref. [6]. The overall effect is a diminishing of the Bragg-scattered intensity. One finds typically for a temperature of 15  $\mu\text{K}$  a DW factor of 0.76. The Bragg beam still has an intensity which exceeds the incoherently scattered background by orders of magnitude. Note that this complication does not affect the symmetry and diagonalization procedure as outlined above. Second, these lattices are still relatively dilute (filling fractions of  $\leq 10\%$ ). This implies a nonperiodic and even time-dependent susceptibility  $\chi$ , due to hopping of atoms from site to site. Therefore the *partial* long-range order (which has been measured in [6]) will accordingly distort the band structure picture.

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