Spectra of electromagnetic excitations in periodic dielectric structures with space and temporal dispersion

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We have studied the influence of space and time dispersion on the frequency dependence of the wave vectors of electromagnetic waves propagating in periodic dielectric structures. Two types of structures are considered: media with weak periodic modulation of the permittivity and photonic crystals composed of periodically arranged identical resonant dielectric particles embedded into nontransparent host medium. It is shown that in these systems, different types of excitations exist, for example, a peculiar kind of polaritons arises in the photonic crystals due to the interaction of the electromagnetic field, eigenoscillations of the dielectric medium, and the Debye resonance. Additional transparency bands and gaps appear in the frequency spectrum of photons due to the dispersion, and their widths depend on the wave vector. The widths of the transparency zones and of the band gaps have been calculated as functions of the frequency and of the parameters of the media. The interaction of different types of waves brings into existence a discontinuity of the frequency at some surfaces in $\vec{k}$ space. If such a surface is not a plane, the classical Bragg condition does not hold.

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I. INTRODUCTION

Propagation of waves in periodic media is a topic of profound importance, both for understanding the general properties of matter-radiation interactions and for the ever-increasing number of practical applications (for example, photonic crystals).[1–3] In spite of the close similarity to the quantum-mechanical problem of electrons in a crystal lattice, the propagation of classical waves in periodic structures exhibits many rather unusual distinctive features. The most dramatic example of such a difference is the effect of time and space dispersion. While the propagation of electromagnetic waves in homogeneous dispersive media has been thoroughly investigated,[4] the effect of dispersion on the radiation propagating in periodic structures remains to be studied in more detail. The exceptions are periodic multiple-quantum-well structures (periodic arrays of dielectric layers), for which the polariton spectrum and the optical response have been studied in Refs. 5 and 6. In Ref. 7, the exciton-polariton susceptibility matrix was calculated, taking into account the well-well interaction, and the polariton dispersion curves have been computed for an infinite periodic array of quantum wells. Some interesting polariton-induced effects were discovered. However, the one dimensionality of the system considered prevented the investigation of important effects present only in dispersive media of higher dimensions.

In the present paper, we deal with the linear wave equation of general type and study the spectral properties of dispersive periodic dielectric structures, namely, the effect of time and space dispersion on the frequency dependence of the wave vector. The employed methods (small perturbation, local perturbation methods, and tight-binding model) impose no restrictions on the dimensionality of the system. As formulated, the problem is closely related to the calculation of the energy of an electron as a function of the wave vector in periodic crystals, although the solution of the corresponding dispersion equation for electromagnetic waves can have several branches, i.e., different types of waves can propagate. Examples are transverse and longitudinal waves in crystal dielectrics with several atoms in the unit cell (e.g., quartz); polaritons in ion crystals; plasma, helicoidal, Alfvén, and cyclotron waves in semiconductors (e.g., InSb); etc. The interaction of these waves is a crucial factor in the formation of the photonic spectrum and gives rise to the appearance of transparency zones and gaps.

The propagation of electromagnetic waves in periodic media is described by Maxwell's equations and the constitutive laws. We first consider a general form of the scalar wave equation as

$$\hat{H}\left(\frac{\partial}{i\partial\vec{r}},-\frac{\partial}{i\partial t}\right)E+\hat{h}\left(\vec{r},\frac{\partial}{i\partial\vec{r}},-\frac{\partial}{i\partial t}\right)E=0, \tag{1}$$

where $\hat{H}$ and $\hat{h}$ are arbitrary functions of $\frac{\partial}{i\partial\vec{r}}$ and $-\frac{\partial}{i\partial t}$, and $\hat{h}$ is a periodic function of $\vec{r}$ with the basic periods $\vec{r}_1$, $\vec{r}_2$, and $\vec{r}_3$ in the x, y, and z directions, respectively. According to the Bloch theorem, the solution of this equation has the form

$$E(\vec{r},t)=\tilde{E}(\vec{r})e^{i[\vec{k}\vec{r}-\omega(\vec{k})t]}, \tag{2}$$

where $\tilde{E}(\vec{r})$ is a periodic function with periods $\vec{r}_1$, $\vec{r}_2$, and $\vec{r}_3$. In nondispersive media, Eq. (1) becomes the classical second-order wave equation; space-time dispersion corresponds to higher-order derivatives with respect to coordinates and time in Eq. (1).

Our goal is to investigate the spectrum of waves propagating in the periodic system, i.e., to find the dependence of the frequency ω on the wave vector $\vec{k}$. Periodic functions $\tilde{E}(\vec{r})$ and $\hat{h}(\vec{r},\frac{\partial}{i\partial\vec{r}},\omega)$ can be expanded in the Fourier series,

$$\tilde{E}(\vec{r})=\sum_{-\infty<n<\infty}\tilde{E}_n e^{i\vec{k}_n\vec{r}}, \tag{3}$$

$$\hat{h}\left(\vec{r},\frac{\partial}{i\partial\vec{r}},\omega\right)=\sum_{n'\neq 0} e^{i\vec{k}_{n'}\vec{r}}h_{n'}\left(\frac{\partial}{i\partial\vec{r}},\omega\right), \tag{4}$$

where $\vec{k}_n$ and $\vec{k}_{n'}$ are the vectors of the reciprocal lattice multiplied by 2π. Without loss of generality, the term h_0 can be set zero by the corresponding renormalization of H.

Substituting Eqs. (2)–(4) in Eq. (1) and setting the coefficients at each $e^{i\vec{\kappa}_n\vec{r}}$ equal zero, we obtain the following infinite system of equations:

$$H(\vec{\varkappa}_m,\omega)\tilde{E}_m+\sum_{-\infty<n<\infty} h_{m-n}(\vec{\varkappa}_n,\omega)\tilde{E}_n=0, \tag{5}$$

$$\vec{\varkappa}_n=\vec{k}+\vec{k}_n. \tag{6}$$

This system of equations has nontrivial solutions $\tilde{E}_n$ if its determinant $D(\vec{\kappa}_m,\omega)$ vanishes,

$$D(\vec{\varkappa}_m,\omega)=0. \tag{7}$$

Equation (7) is the dispersion equation that determines $\omega(\vec{k})$, which is a periodic function with the periods $\vec{k}_n$.[8,9] In what follows, we consider two types of periodic structures: media with weak periodic modulation of the dielectric constant and photonic crystals composed of periodically arranged identical resonant dielectric particles.

II. WEAK PERIODIC MODULATIONS

In this section, we study systems with a weakly modulated dielectric permittivity, so that the second (periodic) term in Eq. (1) can be considered as a small perturbation. This formulation of the problem corresponds, for example, to a photonic crystal, in which the dielectric contrast between the host medium and the elements that form the periodic grating is small. We use the method of Bethe,[10] which enables us to find the frequency spectrum $\omega(\vec{k})$, taking into account multiple scattering.[1,11–13]

When $\hat{h}=0$ (homogeneous medium), from Eq. (1) it follows that $E(\vec{r},t)=E_0e^{i[\vec{k}\vec{r}-\omega(\vec{k})t]}$, and the dispersion equation has the form

$$H(\vec{k},\omega(\vec{k}))=0. \tag{8}$$

Obviously, Eq. (8) follows also from Eq. (5) when all coefficients h_{m-n} are zero, $\tilde{E}_m=0$ for $m>0$, $\tilde{E}_0\neq 0$, and $\vec{k}_0=0$.

Note that only real solutions of Eq. (8), $\omega=\omega_{0l}(\vec{k})$, correspond to propagating waves. We denote the number of such waves by L.

From Eq. (8), it follows that $H(\vec{k},\omega)$ can be rewritten in the form

$$H[\vec{k},\omega(\vec{k})]=f[\vec{k},\omega(\vec{k})]\prod_{l=1}^{L}[\omega-\omega_{0l}(\vec{k})], \tag{9}$$

where $\omega_{0l}(\vec{k})$ are the real roots of Eq. (8) and function f has no roots on the real axis.

If

$$\alpha\equiv\left|\frac{h_n(\vec{k},\omega)}{H(\vec{\varkappa}_n,\omega)}\right|\ll 1, \tag{10}$$

the amplitudes $\tilde{E}_n$ can be found in the first order of small α by setting to zero all $\tilde{E}_n$ with $n>0$ in the second term in Eq. (5), which yields

$$\tilde{E}_n=-\frac{h_n(\vec{k},\omega)}{H(\vec{\varkappa}_n,\omega)}\tilde{E}_0. \tag{11}$$

Setting $m=0$ in Eq. (5) and using expression (11), we get the following dispersion equation for $\omega(\vec{k})$:

$$H(\vec{k},\omega)-\sum_{n\neq 0}\frac{h_{-n}(\vec{\varkappa}_n,\omega)h_n(\vec{k},\omega)}{H(\vec{\varkappa}_n,\omega)}=0. \tag{12}$$

If we write the solutions of Eq. (12) as

$$\omega_l(\vec{k})=\omega_{0l}(\vec{k})+\delta\omega_l(\vec{k})\quad (l=1,\ldots,L) \tag{13}$$

and assume that for all noninteracting waves

$$|\omega_{0l}(\vec{k})-\omega_{0m}(\vec{k})|\gg|\delta\omega_m(\vec{k})|, \tag{14}$$

the corrections $\delta\omega_l(\vec{k})$ can be found by successive approximations. This procedure yields

$$\delta\omega_l(\vec{k})=\frac{1}{f(\vec{k},\omega_{0l})\prod_{m\neq l}^{L}[\omega_{0l}-\omega_{0m}(\vec{k})]}\sum_{n\neq 0}\frac{h_{-n}(\vec{\varkappa}_n,\omega_{0l})h_n(\vec{k},\omega_{0l})}{H(\vec{\varkappa}_n,\omega_{0l})}. \tag{15}$$

Note that these corrections are of the second order in the small periodic perturbation h.

There are at least two cases when the solution Eq. (15) breaks down. Each of them corresponds to a kind of degeneration of the unperturbed solutions and is noticeable for the fact that the periodic modulation lifts the degeneration and brings into existence gaps in the photonic frequency spectrum.

The first case takes place when there exists a domain (a surface S_α) in $\vec{k}$ space where some solution $\omega_{0\alpha}(\vec{k})$ of Eq. (8) coincides with a solution $\omega_{0\beta}(\vec{k})$, and therefore the right-hand side of Eq. (15) diverges because the factor $[\omega-\omega_{0\beta}(\vec{k})]$ in the denominator is zero. In the vicinity of this surface, selecting in Eq. (9) the terms with $l=\alpha,\beta$, we obtain the following dispersion equation:

$$[\omega-\omega_{0\alpha}(\vec{k})][\omega-\omega_{0\beta}(\vec{k})]-\eta_\alpha^2=0, \tag{16}$$

where

$$\eta_\alpha^2=\left\{\frac{1}{f(\vec{k},\omega)\prod\limits_{l\neq\alpha,l\neq\beta}^{L}[\omega-\omega_{0l}(\vec{k})]}\sum_{n\neq 0}\frac{h_{-n}(\vec{\varkappa}_n,\omega)h_n(\vec{k},\omega)}{H(\vec{\varkappa}_n,\omega)}\right\}_{\omega=\omega_{0\alpha}(\vec{k}\in S_\alpha)}. \tag{17}$$

Two solutions of Eq. (16) are

$$\omega_{\alpha,\beta}(\vec{k})=\frac{\omega_{0\alpha}(\vec{k})+\omega_{0\beta}(\vec{k})}{2}\pm\sqrt{\frac{[\omega_{0\alpha}(\vec{k})-\omega_{0\beta}(\vec{k})]^2}{4}+\eta_\alpha^2}. \tag{18}$$

It means that due to the periodic modulation, the frequency as a function of $\vec{k}$ has discontinuity at the surface

$$\omega_{0\alpha}(\vec{k})=\omega_{0\beta}(\vec{k}), \tag{19}$$

i.e., there is a band gap with the half-widths $\eta_\alpha \ll \omega_{0\alpha}(\vec{k})$ in the photonic frequency spectrum. Obviously, a gap exists if η_α is real, $\eta_\alpha^2>0$. Note that the width of the gap is of the first order in the small periodic perturbation h.

Interestingly, when $\omega_{0\alpha}(\vec{k})=\omega_{0\beta}(\vec{k})\equiv\omega_0(\vec{k})$, it might be possible that $\omega_0(\vec{k}_1)+\eta(\vec{k}_1)<\omega_0(\vec{k}_2)-\eta(\vec{k}_2)$ for some $\vec{k}_1$ and $\vec{k}_2$, i.e., the lower edge of the gap at $\vec{k}_2$ overlapped with the upper edge of the gap at $\vec{k}_1$. It means that there is no gap in the spectrum although $\eta\neq 0$.

In the isotropic case, $\omega(\vec{k})\equiv\omega(k^2)$, the surface given by Eq. (19) is a sphere, $k^2=R_\alpha^2$, whose radius R_α is the solution of the equation $\omega_{0\alpha}(k^2)=\omega_{0\beta}(k^2)$. It may take place, for example, in the plasma of a semiconductor (such as A_3B_5), in which case α and β correspond to the transverse and longitudinal (plasma) waves, respectively.

The small perturbation solution [Eq. (11)] is invalid in areas where the frequency ω is close to one of the roots (say, root number p) of the equation $H(\vec{\kappa}_n,\omega)=0$. In this instance, we get back to Eq. (5) and, following Ref. 11, keep there only two terms with $m=0$, p, whereupon the dispersion equation takes the form

$$H(\vec{k},\omega)H(\vec{\varkappa}_p,\omega)-h_p(\vec{k},\omega)h_{-p}(\vec{\varkappa}_p,\omega)=0. \tag{20}$$

If there is a region in the $\vec{k}$ space in which $\omega_{0a}(\vec{k})=\omega_{0b}(\vec{\varkappa}_p)$ for two different types of waves (a and b), using for $H(\vec{k},\omega)$ and $H(\vec{\varkappa}_p,\omega)$ the presentation Eq. (9) and separating out terms with $l=a,b$, from Eq. (20) we obtain

$$[\omega-\omega_{0a}(\vec{k})][\omega-\omega_{0b}(\vec{\varkappa}_p)]-\zeta_{\alpha p}^2=0, \tag{21}$$

where

$$\zeta_{ap}^2=\left\{\frac{h_p(\vec{k},\omega)h_{-p}(\vec{\varkappa}_p,\omega)}{f(\vec{k},\omega)f(\vec{\varkappa}_p,\omega)\prod\limits_{l=1,l\neq a}^{L}[\omega-\omega_{0l}(\vec{k})]\prod\limits_{l=1,l\neq b}^{L}[\omega-\omega_{0l'}(\vec{\varkappa}_p)]}\right\}_{\omega=\omega_{0a}(\vec{k}\in S_a)}. \tag{22}$$

The solution of Eq. (21) is given by Eq. (18) with $\alpha=a$, $\beta=b$, and $\eta=\zeta$. At surfaces S_a given by the equation $\omega_{0a}(\vec{k})=\omega_{0b}(\vec{\varkappa}_p)$, the frequency has discontinuities and gaps appear. Obviously, ζ_{ap} is the half-width of the periodicity-induced band gap in the photonic frequency spectrum.

In the isotropic case, the equation of the surfaces S_a becomes

$$\omega_{0a}(k^2)=\omega_{0b}(\varkappa_p^2). \tag{23}$$

If $a=b$, from Eq. (23), it follows that

$$k^2=\varkappa_p^2,$$

or

$$2\vec{k}\vec{k}_p=-k_p^2. \tag{24}$$

For each p, Eq. (24) (Bragg condition) is the equation of a plane, which is the boundary of the corresponding Brillouin zone.[9]

If $a\neq b$, from Eq. (23), if follows that at small k^2 and $\varkappa_p^2$, the equation of the surface at which the frequency has a discontinuity takes the form

$$(\vec{k}-\vec{q}_{ab})^2=k_{ab}^2, \tag{25}$$

where

$$\vec{q}_{ab}=\frac{\omega_{0b}'(0)}{\omega_{0a}'(0)-\omega_{0b}'(0)}\vec{k}_b,$$

$$k_{ab}^2 = \frac{\omega_{0a}'(0)\omega_{0b}'(0)}{[\omega_{0a}'(0) - \omega_{0b}'(0)]^2} k_b^2 + \frac{\omega_{0b}(0) - \omega_{0a}(0)}{\omega_{0a\alpha}'(0) - \omega_{0b}'(0)},$$

$$\omega_{0a}' = \frac{\partial \omega_{0a}(0)}{\partial k^2}, \quad \omega_{0b}' = \frac{\partial \omega_{0b}(0)}{\partial k_b^2}. \tag{26}$$

Equation (25) is the equation of a sphere with the center at the point $\vec{q}_b$ and radius k_{ab}.

Thus, from the results of this section, it follows that the interference of the dispersion-induced waves in a periodically modulated medium brings into existence additional (as compared to nondispersive periodic media) surfaces in $\vec{k}$ space, on which the frequency as a function of the wave vector, $\omega(\vec{k})$, exhibits discontinuity and therefore band gaps appear. The shape of these surfaces depends on the parameters of the medium, in contrast to the boundaries of the conventional Brillouin zones that are determined solely by the symmetry of the system.

III. PERIODIC ARRAY OF RESONANT PARTICLES

In what follows, we consider a photonic crystal comprised of identical dielectric particles periodically arranged in a nontransparent medium with negative dielectric constant, $\varepsilon_0 < 0$, and study the spectrum of excitations (eigenwaves) associated with the resonances of a single particle.

A. Local perturbation method

In this section, we consider the frequency range where the typical size d of the particles is small so that

$$d \ll \frac{2\pi c}{\sqrt{|\varepsilon_0|}\omega}. \tag{27}$$

In this instance, the problem can be handled by the local perturbations method (LPM) originally developed by Fermi.[14] The method is widely used in the theory of disordered media,[15] the theory of crystals,[5] and electrodynamics.[16–19] LPM is based on the assumption that the (unknown) field is independent of the coordinates inside each particle. In contrast to the Born approximation, which considers only weak scattering, LMP is valid for arbitrarily large amplitudes of the scattered fields and does not rule out the existence of resonances that take place when d is of order of the wavelength inside the particle ($d \sim \frac{2\pi c}{n\omega}$, where n is the dielectric constant of the particle).

In this case, Eq. (1) takes the form

$$\hat{H}\left(\frac{\partial}{i\partial\vec{r}}, -\frac{\partial}{i\partial t}\right)E + \sum_{n=-\infty}^{\infty} U\left(\vec{r} - \vec{r}_n, -\frac{\partial}{i\partial t}\right)E = 0, \tag{28}$$

where the space-time dispersion of the homogeneous host medium is incorporated in $\hat{H}$, and U is nonzero only inside the particles and describes their shape, positions, and dielectric properties [see, for example, Eq. (42) below]. For the sake of simplicity, in what follows, we assume that the dielectric particles possess only time dispersion.

Obviously, the sum in Eq. (28) is a periodic function of $\vec{r}$. Therefore, the solution of Eq. (28) can be presented in the form of Eq. (2). If inequality (27) holds, the LPM approximation is applicable, which means that

$$U(\vec{r} - \vec{r}_n, \omega)E(\vec{r})e^{i\vec{k}\vec{r}} \approx U(\vec{r} - \vec{r}_n, \omega)\tilde{E}(\vec{r}_n)e^{i\vec{k}\vec{r}_n}. \tag{29}$$

$\tilde{E}(\vec{r})$ is a periodic function, and if we assume that one of the particles is located at the origin, $\vec{r}=0$, then $\tilde{E}(\vec{r}_n)=\tilde{E}(0)$. Substitution of Eq. (29) into Eq. (28) yields

$$\hat{H}\left(\frac{\partial}{i\partial\vec{r}}, \omega\right)E(\vec{r}) + \tilde{E}(0)\sum_{n=-\infty}^{\infty} U(\vec{r} - \vec{r}_n, \omega)e^{i\vec{k}\vec{r}_n} = 0. \tag{30}$$

Equation (30) can be rewritten in the integral form as

$$E(\vec{r}) + \tilde{E}(0)\sum_n e^{i\vec{k}\vec{r}_n} \int G(\vec{r} - \vec{r}\,')U(\vec{r} - \vec{r}_n, \omega)d\vec{r} = 0, \tag{31}$$

where the Green's function of the homogeneous ($U=0$) host medium, $G(\vec{r}, \omega)$, is defined by the equation

$$\hat{H}\left(\frac{\partial}{i\partial\vec{r}}, \omega\right)G(\vec{r}, \omega) = \delta(\vec{r} - \vec{r}\,'), \tag{32}$$

whose solution is

$$G(\vec{r} - \vec{r}\,') = \frac{1}{(2\pi)^3}\int \frac{e^{i\vec{k}(\vec{r}-\vec{r}\,')}}{H(\vec{k}, \omega)}d\vec{k}. \tag{33}$$

Setting $\vec{r}=0$ in Eq. (31), we obtain the following dispersion equation for $\omega(\vec{k})$:

$$1 + \int G(\vec{r}\,')U(\vec{r}\,')d\vec{r}\,' + \int U(\vec{r}\,')d\vec{r}\,' \sum_{n\neq 0} G(\vec{r}\,' + \vec{r}_n)e^{i\vec{k}\vec{r}_n} = 0. \tag{34}$$

It is apparent that the second term in Eq. (34) corresponds to an isolated single particle, while the third term accounts for the corrections due to the interparticle interaction. If the typical distance between particles is larger than the "wavelength" in the host medium, these corrections are small compared to the second term. Therefore, we seek the solutions of Eq. (34) as

$$\omega_p = \omega_{0p} + \delta\omega_p, \tag{35}$$

where p is the index of a solution, ω_{0p} are the eigenfrequencies of a single particle in the host medium, i.e., the solutions of the "zero-order" (without interaction) equation,[17]

$$1 + \int G(\vec{r}\,', \omega)U(\vec{r}\,', \omega)d\vec{r}\,' = 0, \tag{36}$$

and $\delta\omega_p \ll \omega_{0p}$.

In an isotropic medium, H depends on k^2 and $G(\vec{r}-\vec{r})$ is equal to

$$G(\vec{r}-\vec{r}\,') = \frac{1}{4\pi|\vec{r}-\vec{r}\,'|}\sum_{l=1}^{L}\frac{e^{-\varkappa_l|\vec{r}-\vec{r}\,'|}}{H'(-\varkappa_l^2)}, \tag{37}$$

where $\varkappa_l=|\vec{k}_l|$, $H'(-\varkappa_l^2)=\frac{dH(-\varkappa_l^2)}{d\varkappa_l^2}$, and $\varkappa_l^2$ are the roots of the equation

$$H(\varkappa^2,\omega)=0. \tag{38}$$

Our concern is only with real frequencies. Therefore, $G(\vec{r}-\vec{r})$ should be a real function (this is the necessary but not sufficient condition) and, consequently, the roots $\varkappa_l^2$ of Eq. (38) should be imaginary and $H'(\varkappa^2,\omega)$ real quantities.

Since the summands in Eq. (34) decrease exponentially with increasing $|\vec{r}_n|$, we keep only the term with the minimal $\varkappa_l$ (denote it by $\bar{\varkappa}$). Then, for $\delta\omega_p$, we find

$$\delta\omega_p = \left\{-\frac{\int U(\vec{r}\,')d\vec{r}\,'}{\frac{d}{d\omega}\int G(\vec{r}\,',\omega)U(\vec{r}\,',\omega)d\vec{r}\,'}\frac{1}{4\pi}\sum_{n\neq 0}\frac{\exp(-\bar{\varkappa}|\vec{r}_n|)}{H'(-\bar{\varkappa}^2)|\vec{r}_n|}e^{i\vec{k}\vec{r}_n}\right\}_{\omega=\omega_{0p}}. \tag{39}$$

For the same reason, in the sum in Eq. (39), we take into account only the terms corresponding to the interaction with the nearest neighbors. For a crystal with a cubic cell of the linear size b, it yields

$$\delta\omega_p = A(\cos k_x b + \cos k_y b + \cos k_z b). \tag{40}$$

$$A = -\left\{\frac{\int U(\vec{r}\,')d\vec{r}\,' e^{-\bar{\varkappa}b}}{2\pi b H'(-\bar{\varkappa}^2)\frac{d}{d\omega}\int G(\vec{r},\omega)U(\vec{r},\omega)d\vec{r}}\right\}_{\omega=\omega_{0p}}. \tag{41}$$

It means that the resonant frequencies of a single particle broadens (due to the interaction between the neighboring particles) and form passing zones of finite widths Δ_p, i.e., although the host medium is opaque, the crystal is transparent at the frequencies inside there zones.

To carry out the integration in Eq. (39), we consider an example of a homogeneous medium with time dispersion. In this instance, the operator $\hat{H}$ in Eq. (38) is the Helmholtz operator

$$\hat{H} = \Delta + \frac{\omega^2}{c^2}\varepsilon_0(\omega), \tag{42}$$

where $\varepsilon_0(\omega)$ is the dielectric permittivity of the host medium, in which the periodic grating of particles (local perturbations) is located. If, for example, the dielectric constants of both host medium and particles are of the Drude form,

$$\varepsilon_0(\omega) = 1 + \frac{\Omega_0^2}{\nu_0^2-\omega^2}, \tag{43}$$

$$\varepsilon(\omega) = 1 + \frac{\Omega_1^2}{\nu_1^2-\omega^2}, \tag{44}$$

where ν_0 and ν_1 are eigenfrequencies of the media and Ω_0 and Ω_1 are the corresponding plasma frequencies.

The dispersion equation [Eq. (36)] has two solutions,

$$\omega_{01,02}^2 = \frac{\Omega_1^2+\nu_1^2+\nu_s^2}{2} \pm \sqrt{\left(\frac{\Omega_1^2+\nu_1^2+\nu_s^2}{2}\right)^2 - \nu_1^2\nu_s^2}, \tag{45}$$

where

$$\nu_s^2 = \frac{4\pi c^2}{S}$$

is the frequency of the "geometrical" resonance related to the finite size d of the local perturbation (Debye resonance of a single particle), and

$$S = \int \frac{f(\vec{r})d\vec{r}}{r} \sim d^2.$$

Note that the number of solutions depends on the explicit form of the function $\varepsilon_0(\omega)$ and can be more than 2.

Frequencies $\omega_{1,2}=\omega_{01,02}+\delta\omega_{1,2}$ correspond to a peculiar kind of polaritons that arise in the photonic crystal with time dispersion due to the interaction of the electromagnetic field (ω), eigenoscillation of the dielectric medium (υ_1), and Debye resonance (ν_s).

Recall that for the exponent in the Green's function to be real, it is necessary that

$$\omega_{1,2}^2 > \upsilon_0^2 + \Omega_0^2 \equiv \Omega^2.$$

If, for example, three frequencies ν_s, υ_1, and Ω_1 are of the same order of magnitude, the widths of the passing zones $\Delta_{1,2}$, are

$$\Delta_{1,2} \sim e^{-\bar{\varkappa}b}\frac{d}{b}\omega_{1,2}. \tag{46}$$

The zone width is maximal at $\omega_{1,2}=\Omega$ and is equal $\Delta_{1,2} \sim \frac{d}{b}\omega_{1,2}$. With $\frac{\Omega^2}{\omega_{01,2}^2}$ increasing, the width decreases exponentially, and at $\frac{\Omega^2}{\omega_{01,2}^2} \gg 1$, the zone structure disappears. As the spacing between levels, $|\omega_1-\omega_2|$, is of the order of ω_s, the width of the passing zone is $\frac{b}{d}\gg 1$ times smaller than the size of the band gap.

It should be remembered that the results of this subsection have been obtained in the framework of the local perturbation method and, therefore, are valid only when the characteristic size d of the particles that form the photonic crystal is smaller than the wavelength of the radiation in the host medium.

B. Tight-binding model

A weakness of LPM is that it enables one to obtain only the lowest eigenfrequencies determined solely by the volume of the single particle. Below, we present the tight-binding approximation,[12] which is not subject to this limitation. We use it in combination with the Galerkin method[20] to calculate the frequency spectrum of a periodic array of dielectric particles with positive dielectric constant located at points $\vec{r}_n$ in a medium with negative dielectric constant. From the physical standpoint, these particles constitute a system of connected resonators.

We assume that the set of the resonant frequencies ω_{0m} and the corresponding eigen-wave-functions $E_{0m}(\vec{r},\omega_{0m})$ of a single resonator are known and the overlap of the wave functions of the neighboring particles is weak. This means that the eigenfrequencies of the periodic array can be presented as $\omega_m=\omega_{0m}+\delta\omega_m$, where $\delta\omega_m\ll\omega_{0m}$. Substituting $-\frac{\partial}{i\partial t}=\omega_{0m}+\delta\omega_m$ in Eq. (28) and expanding it up to the first order of the small parameter $\frac{\delta\omega_m}{\omega_{0m}}$, we obtain

$$\hat{H}\left(\omega_{0m},-\frac{\partial}{i\partial\vec{r}}\right)E(\vec{r})+\frac{\partial\hat{H}\left(\omega_{0m},-\frac{\partial}{i\partial\vec{r}}\right)}{\partial\omega_m}\delta\omega_m E(\vec{r})+\sum_n U\left(\omega_{0m},\vec{r}-\vec{r}_n,\frac{\partial}{i\partial\vec{r}}\right)E(\vec{r})=0. \tag{47}$$

The essence of the Galerkin method lies in replacing the unknown function $E(\vec{r})$ by a sampling function, which, for the periodic system under consideration, we choose to be

$$E(\vec{r})=\sum_{n=-\infty}^{\infty}e^{i\vec{k}\vec{r}_n}E_0(\vec{r}-\vec{r}_n,). \tag{48}$$

An advantage of this choice is that this function, which is of the Bloch type, is equal (within the factor $e^{i\vec{k}\vec{r}_n}$) to $E_0(\vec{r})$ at the sites of the crystal lattice and decreases away from the particles. Substituting Eq. (48) into Eq. (47), multiplying it by $E_0(\vec{r}-\vec{r}_n)$, and integrating over volume, we obtain

$$\delta\omega_m=\frac{J_{10}+\sum_{\substack{n=-\infty\\n\neq0}}^{\infty}J_{1n}e^{i\vec{k}\vec{r}_n}}{J_{20}+\sum_{\substack{n=-\infty\\n\neq0}}^{\infty}J_{2n}e^{i\vec{k}\vec{r}_n}}, \tag{49}$$

where

$$J_{1n}=\int E_0(\vec{r})\hat{h}\left(\omega_{0m},\vec{r},-\frac{\partial}{i\partial\vec{r}}\right)E_0(\vec{r}-\vec{r}_n)d\vec{r}, \tag{50}$$

$$\hat{h}=\sum_{p\neq m}U\left(\omega_{0m},\vec{r}-\vec{r}_p,-\frac{\partial}{i\partial\vec{r}}\right),$$

$$J_{2n}=\int E_0(\vec{r})\frac{\partial\hat{H}_0\left(\omega_{0m},\frac{\partial}{\partial\vec{r}}\right)}{\partial\omega}E_0(\vec{r}-\vec{r}_n)d\vec{r}. \tag{51}$$

Under assumption of weak overlap of the eigen-wave-functions of the neighboring particles, Eq. (49) becomes

$$\delta\omega_m=\frac{1}{J_{20}}\sum_n^{\infty}J_{1n}e^{i\vec{k}\vec{r}_n}. \tag{52}$$

Taking into account only terms corresponding to the interaction with the nearest neighbors, for a crystal with cubic cell, we obtain

$$\delta\omega_m=\frac{J_{10}}{J_{20}}+2\frac{J_{11}}{J_{20}}(\cos k_x b+\cos k_y b+\cos k_z b). \tag{53}$$

The width of the passing zone is therefore equal to $12\frac{J_{11}}{J_{20}}$.

Note that in the tight-binding approximation, the width of a passing zone is determined by the overlap of the eigen-wave-functions, while in LPM (previous section), it was specified by the unperturbed Green's function. In contrast to LPM, the applicability of the tight-binding approximation does not impose any restrictions on the ratio between the wavelength and the size of particles. On the other hand, LPM makes compact analytical expressions possible, whereas the overlapping integrals are usually calculated numerically.

To conclude, the frequency spectra of electromagnetic waves have been studied in continuous media with periodically modulated dielectric permittivity, in photonic crystals comprised of periodically arranged particles whose size is small compared to the wavelength of the radiation in the host medium, and in a periodic array of optical resonators with weakly overlapping wave functions. The methods and most of the results are rather general and are applicable to any dimension, type of dispersion, and shape of the particles. It is shown that time-space dispersion causes important differences between the spectrum of photons in periodic dielectric systems and that of electrons in solid-state crystals. For example, a peculiar type of polaritons exists in photonic crystals due to the interplay between the electromagnetic field, eigenoscillations of the medium, and the Debye resonance. The dispersion increases the number of the transparency bands and deforms dramatically the shape of their boundaries and leads to the dependence of the width of the gaps in the frequency spectrum of photons on the wave vector.

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