A study of a phase formalism for calculating the cumulative density of states of one-dimensional photonic crystals

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ABSTRACT

We explore a phase formalism that underpins a method of calculation of the cumulative density of states of one-dimensional photonic crystals based on the node-counting theorem. Node counting is achieved by considering the spatial dependence of a phase variable proportional to the logarithmic derivative of the electric field in the structure. The properties of the phase variable are considered for photonic crystals in general, and illustrative algebraic and numerical results are presented for the phase variable and cumulative density of states of a model crystal. It is also shown how a simple extension of the theory can facilitate the calculation of the reflectivity of finite samples. For a disordered model crystal, a differential equation for the distribution function of the phase variable is derived and then used to obtain a closed-form expression for the ensemble-averaged cumulative density of states and numerical results to illustrate band tailing in the photonic bandgap.

KEYWORDS
Photonic crystal; phase formalism; node counting; cumulative density of states; disorder

1. Introduction

The cumulative (or integrated) density of states of a photonic structure for a given frequency is the number of electromagnetic states per unit volume with frequency less than that value. Greshnov et al (*1*, *2*) have reported calculations of the cumulative density of states of one-dimensional disordered photonic crystals based on the node-counting theorem (*3*–*5*), which has a well-documented history of use in numerical and analytical calculations of the density of states as a function of energy of a quantum particle in a one-dimensional random potential (see for example the original work of (*4*–*6*) and the reviews of (*7*, *8*)).

One approach to counting nodes in the quantum problem is to define a phase (*6*, *8*) in terms of the logarithmic derivative of real wavefunctions of the system. In a disordered system that phase can be treated as a stochastic variable whose probability distribution can be used to determine the cumulative density of states. Greshnov et al

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(*1*, *2*) were the first to use an analogous approach to calculate the density of photonic states of a disordered one-dimensional photonic crystal. They considered a structure consisting of equal-thickness alternating layers of two different dielectric materials where some randomness was introduced into the values of the refractive indices of the layers. With the aid of some judicious approximations they were able to derive a Fokker-Planck equation (*9*) for the distribution function of the phase and then solve that equation to predict the density of states at frequencies in and close to the lowest-frequency bandgap of the structure. In later work (*10*) the light localization length was studied using similar techniques.

The main motivation for the work reported in (*1*, *2*) was to provide an analysis of the numerical studies reported in (*11*) of disorder-induced band tailing in the bandgap of a specific type of photonic crystal. While that aim was achieved, constraints of paper length and the focus on a specific problem meant that it was not possible to discuss some additional interesting features of the phase formalism, including its application to calculating the density of states of perfect photonic crystals as well as disordered structures. Therefore in this paper we consider the more general potential of the approach and also describe an in-depth study of the theory of a particular model system with a simplicity that facilitates the analysis and hence allows the discussion to concentrate on further interesting aspects of the phase formalism.

Photonic bandgaps are manifested in the reflection spectrum of a photonic structure and we show in section 4 how the wave admittance of the electromagnetic field in a one-dimensional structure, which is also defined in terms of the logarithmic derivative of the electric field, may be used to advantage in the calculation of the reflectivity of certain crystals.

2. A method for calculating the cumulative density of states of a photonic structure using the phase formalism

We consider the problem of calculating the cumulative density of states of a one-dimensional photonic structure described by a refractive index profile $n(x)$ as a function of position x. Consideration is restricted to states that have spatial variation only in the x-direction. Those states have have orthogonal electric and magnetic fields in the y-z plane and all the calculations presented refer to just one of the two independent field-polarizations that can be chosen.

The method of calculation is based on the node-counting theorem (*3*, *4*, *7*, *8*) which, in the electromagnetic context considered here, states that the number of frequency eigenvalues of the wave equation not exceeding any given angular frequency ω in a system of given length does not differ by more than unity from the number of zeroes of the electric field at frequency ω when it has a real logarithmic derivative at one end of the system. However, it should be noted that the electric field functions calculated with such a boundary condition will not normally be eigenfunctions of the wave equation.

Using the complex notation, we consider electric fields that have a dependence on x and time t of the form $E(x)\exp[i(\omega t+\delta)]$, where $E(x)$ is a *real* function of position and δ is a phase constant. Then the problem reduces to counting the number of zeroes in the function $E(x)$ as a function of ω. To count the zeroes in the electric field it is convenient to consider a dimensionless quantity proportional to the logarithmic derivative of the electric field:

$$X(x) = \frac{\alpha/k_0}{E(x)} \frac{dE(x)}{dx}, \tag{1}$$

where $k_0 = \omega/c$ (with c the velocity of light) and α is a constant. At each zero in $E(x)$ there will be a divergence in $X(x)$ and the counting of those is facilitated by writing

$$X(x) = \cot(\phi(x)/2). \tag{2}$$

It is apparent from equation 2 that the zeroes in $E(x)$ occur when the phase variable $\phi(x) = 0, \pm 2\pi, \pm 4\pi \ldots$ and hence with uniform density $1/2\pi$ in ϕ-space. It follows that the cumulative density of states per unit length $N(\omega)$ is given by

$$N(\omega) = \left(\phi(x_2) - \phi(x_1)\right)/2\pi(x_2 - x_1) \tag{3}$$

as $x_2 - x_1 \to \infty$. It should be noted that although the detailed behaviour of $\phi(x)$ depends on the choice of the constant α in equation 2, that choice does not affect the values of x at which ϕ becomes an integer multiple of 2π and hence equation 3 for $N(\omega)$ is universally applicable.

It is clear from equation 3 that $N(\omega)$ follows directly from a knowledge of $\phi(x)$. A differential equation determining $\phi(x)$ can be obtained by first deriving the equation obeyed by $X(x)$. From equation 1 we have

$$\frac{dX(x)}{dx} = \frac{\alpha}{k_0}\left(\frac{E\left(d^2E/dx^2\right) - \left(dE/dx\right)^2}{E^2}\right) = -\alpha k_0 n(x)^2 - (k_0/\alpha)X(x)^2, \tag{4}$$

where we have made use of the wave equation for electric field,

$$\frac{d^2E}{dx^2} + n(x)^2 k_0^2 E = 0, \tag{5}$$

in the second equality. Substituting equation 2 into 4 gives a differential equation for the phase $\phi(x)$,

$$\frac{d\phi}{dx} = (k_0/\alpha)\left[\left(1 + \alpha^2 n(x)^2\right) + \left(1 - \alpha^2 n(x)^2\right)\cos\phi\right], \tag{6}$$

which will normally have to be solved numerically.

3. An example of the application of the phase formalism to a model one-dimensional photonic crystal

We begin our study of the application of the phase formalism to the calculation of the cumulative density of states of one-dimensional photonic crystals by considering a simple model of a perfect crystal in which the relative permittivity has a sinusoidal variation with x of fractional amplitude γ and period a about a mean value n_0^2:

$$n(x)^2 = n_0^2\left(1 + \gamma \sin px\right), \tag{7}$$

where $n(x)$ is the refractive index and $p = 2\pi/a$. Equation 7 describes a mathematically convenient model system but we will find that as well as having the virtue of simplicity, it exhibits properties that are common to more practical structures and provides useful theoretical insight into those properties. We consider a particular case of the crystal with $n_0 = 2.5$ and $\gamma = 0.5$, giving a refractive index that oscillates between 1.77 to 3.06. A high dielectric contrast has been chosen to provide a stringent test for the approximations that will be used in the analysis.

Note that with a modulation defined in terms of a continuously varying relative permittivity and a high dielectric contrast, the example considered here is rather different from the structure considered in (*2*) with its step-function modulation of the refractive index and much lower dielectric contrast.

Substituting equation 7 in equation 6, choosing $\alpha = 1/n_0$ and writing $y = px$ gives

$$\frac{d\phi}{dy} = n_0\sigma\left[2 + \gamma \sin y(1 - \cos\phi)\right], \tag{8}$$

where $\sigma = k_0/p = \omega a/2\pi c$. Instead of attempting to solve equation 8 directly there is some advantage in considering the deviation of the phase from the value it would have in a homogeneous medium with the relative permittivity n_0^2, which we will call the effective medium value. The solution to equation 8 when $\gamma = 0$ (so that $n(x) = n_0$) is simply $\phi(y) = 2n_0\sigma y$. Then if we write

$$\phi(y) = 2n_0\sigma y + \theta(y), \tag{9}$$

and substitute ϕ into equation 8, we see that $\theta(y)$ can be determined by solving

$$\frac{d\theta(y)}{dy} = n_0\sigma\,\gamma \sin y\left[1 - \cos(2n_0\sigma y + \theta(y))\right]. \tag{10}$$

It follows from equation 3 that the cumulative density of states *per unit cell* of the structure is given by

$$N_{uc}(\omega) = \frac{\theta(y_2) - \theta(y_1)}{y_2 - y_1} + 2n_0\sigma. \tag{11}$$

The second term in equation 11 contributes a constant linear increase in the cumulative density of states with frequency. Numerical solution of equation 10 shows that the contribution of the first term is relatively small except at the band edges, and in the bandgap where its decrease with frequency exactly cancels the increase given by the first term.

The spatial dependence of θ is shown in figure 1 for $\sigma = 0.1$, corresponding to the middle of the first band, in the region around 100 unit cells from the point $y = 0$ where θ is set to zero as the boundary condition for the calculation. The oscillatory behaviour of θ is superimposed on a slow increase of its mean value, indicating that the cumulative density of states at this frequency is essentially identical to that of a homogeneous medium of refractive index n_0. Because the oscillations have relatively small amplitude about $\theta \approx \pi/2$ they can be reproduced to a good approximation by taking $\theta = \pi/2$ on the right hand side of equation 10 and then integrating over y.

Although there is no net change in phase across the photonic structure in the bandgap, the phase does exhibit spatial oscillations which are frequency-dependent.

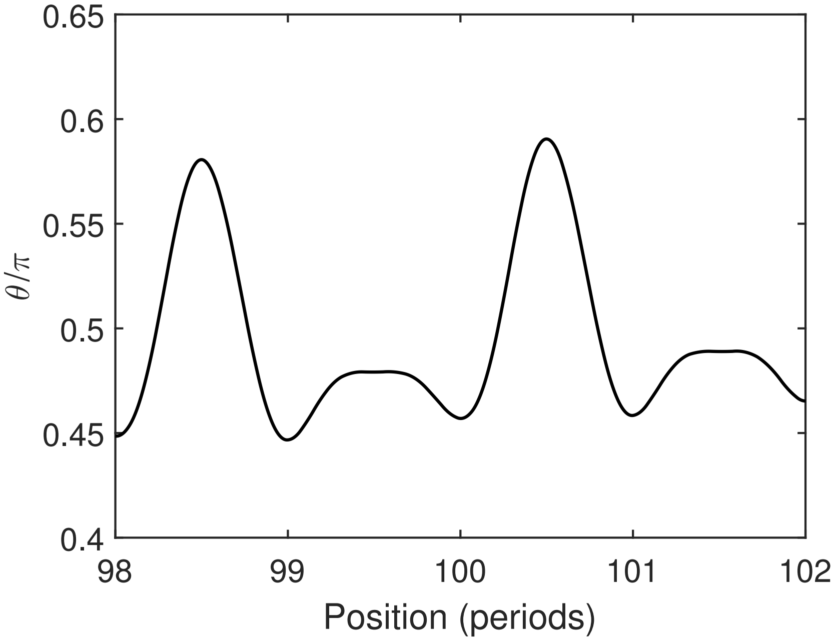

Figure 1. The phase variable θ (defined by equations 2 and 9) as a function of position in four crystal periods in the body of a photonic crystal in which the square root of the mean relative permittivity is $n_0 = 2.5$ and the fractional amplitude of the sinusoidal permittivity modulation is $\gamma = 0.5$. $\sigma = \omega a/2\pi c = 0.1$, which is at the centre of the lowest photonic band.

To study the spatial and frequency dependence of the phase in the bandgap it is instructive to consider how ϕ departs from its effective medium value in the bandgap. Basic diffraction considerations suggest that the first bandgap exists at the wavevector $p/2$ and hence around frequency $\omega \approx \omega_g = \pi c/n_0 a$ and $\sigma \approx 1/2n_0$. Hence we take the effective medium value of $2n_0\sigma y$ to be simply y and write

$$\phi(y) = y + \psi(y) \tag{12}$$

Substituting for ϕ in equation 8 gives

$$\frac{d\psi(y)}{dy} = 2n_0\sigma - 1 + n_0\sigma\,\gamma \sin y\,[1 - \cos(y + \psi(y))]\,. \tag{13}$$

Equation 13 may be solved numerically and figure 2 shows a typical example of how ψ is a periodic function of position inside the bandgap. Figure 3 shows that the mean value of ψ varies with frequency and takes the value π close to the gap centre. Outside the bandgap ψ is no longer periodic and its mean value changes monotonically from unit cell to unit cell.

The cumulative density of states per unit cell may be obtained by numerical solution of equation 13 and then use of

$$N_{uc}(\omega) = \frac{\psi(y_2) - \psi(y_1)}{y_2 - y_1} + 1, \tag{14}$$

which is derived from equation 3, $y = px$ and $\phi(y) = y + \psi(y)$.

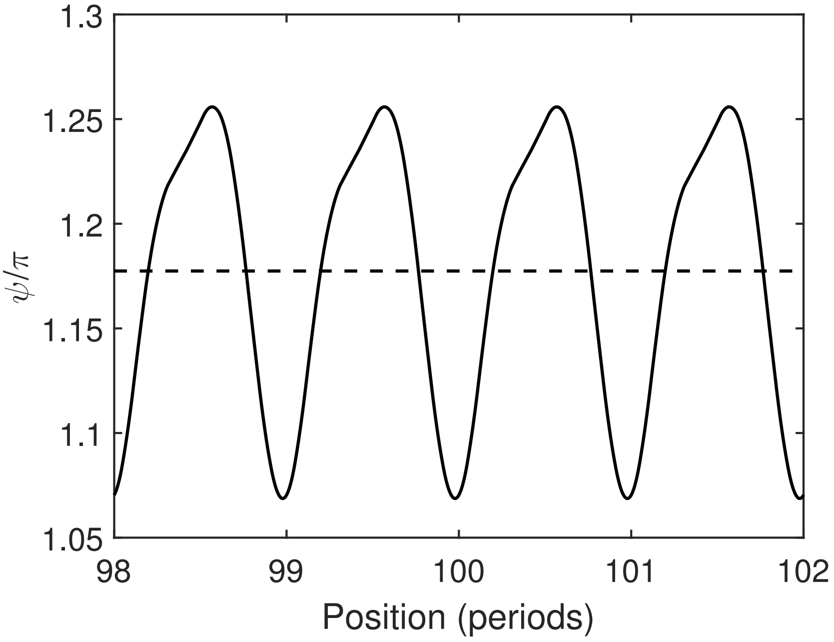

Figure 2. The solid line shows the phase variable ψ (defined by equations 2 and 12) as a function of position in four crystal periods in the body of the structure described in the caption of figure 1. The dashed line shows the mean value of ψ. $\sigma = \omega a/2\pi c = 0.215$, which corresponds to the upper half of the lowest bandgap.

However, equation 13 may be simplified somewhat by using approximations based on the periodicity of the structure and of ψ, and the relatively small amplitude of oscillation of ψ. Expanding the cosine term in equation 13 and neglecting the oscillation of ψ while averaging over a unit cell of the structure gives

$$\frac{d\psi_a}{dy} = F + G\sin\psi_a, \tag{15}$$

where $F = 2n_0\sigma - 1 = (\omega/\omega_g) - 1$, $G = n_0\sigma\,\gamma/2 = (\gamma/4)(\omega/\omega_g)$ and the subscript a on ψ denotes an approximate solution.

For $F^2 \leq G^2$ equation 15 may be integrated (*12*) to give

$$\frac{1}{\sqrt{G^2 - F^2}} \ln\left(\frac{F\tan(\psi_a/2) + G - \sqrt{G^2 - F^2}}{F\tan(\psi_a/2) + G + \sqrt{G^2 - F^2}}\right) = y + A, \tag{16}$$

where A is an arbitrary constant. As $y \to \pm\infty$, $\tan(\psi_a/2) \to -(G \pm \sqrt{G^2 - F^2})/F$ or equivalently

$$\psi_a = \arcsin(-F/G), \tag{17}$$

which when substituted into equation 15 gives $d\psi_a/dy = 0$. Alternatively we could have argued rather more directly that for $F^2 \leq G^2$ there is a real stationary solution to equation 15 that is equation 17. In support of the validity of the approximations made, it is clear from figure 3 that the variation of ψ_a with frequency is very close to the *mean value* of ψ obtained by numerical solution of equation 13.

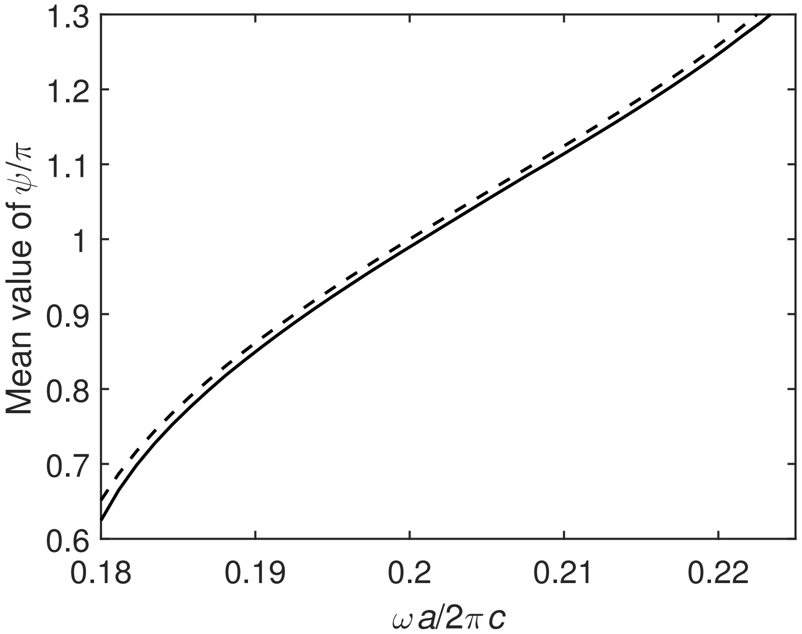

Figure 3. The mean value of the phase variable ψ as a function of the normalized angular frequency $\omega a/2\pi c$ ($=\sigma$) in the first bandgap of the photonic crystal described in the caption of figure 1. The solid curve has been obtained by numerical solution of equation 13 and the dashed curve is ψ_a as defined by equation 17.

Since our approximation to ψ, ψ_a, does not change with y there is no contribution to $N_{uc}(\omega)$ from the first term on the right hand side of equation 14 and $N_{uc}(\omega) = 1$. With no change of the cumulative density of states with ω in the frequency range for which $F^2 \leq G^2$, we can say there is a bandgap. The condition $F^2 = G^2$ gives the edges of the bandgap as

$$\omega = \omega_g \left(1 \pm \frac{\gamma}{4}\right)^{-1} \approx \omega_g \left(1 \mp \frac{\gamma}{4}\right) \tag{18}$$

For $F^2 > G^2$ equation 15 may be integrated (*12*) to give

$$\frac{2}{\sqrt{F^2 - G^2}} \arctan\left(\frac{F\tan(\psi_a/2) + G}{\sqrt{F^2 - G^2}}\right) = y + B, \tag{19}$$

where B is an arbitrary constant. This gives the relationship between ψ_a and y outside the bandgap as long as we interpret the arctan function in a way that allows values of ψ_a over an infinite range instead of just in the interval $(-\pi/2\,, +\pi/2)$ used to define the principal value. However, consideration of only that interval is sufficient to calculate the cumulative density of states. Taking the difference of equation 19 for the cases $\psi_a = \pi$ and $\psi_a = -\pi$ gives

$$y(\pi) - y(-\pi) = 2\pi\,\mathrm{sign}(F)/\sqrt{F^2 - G^2},$$

where sign denotes the signum function. Then the simple result for the cumulative density of states outside the bandgap,

$$N_{uc}(\omega) = 1 + \mathrm{sign}(F)\sqrt{F^2 - G^2}\,, \tag{20}$$

follows from equation 14. The cumulative density of states near the first bandgap predicted by equation 20 is shown by the solid curve in figure 4 and closely reproduces the density of states found from a full numerical solution of equation 13.

For frequencies sufficiently close to the upper edge of the lowest band we can expand $F^2 - G^2$ in equation 20 about the frequency of the bandgap edge given by equation 18, which we denote by ω_{be}. For the case of $\gamma = 0.5$ considered here we can then derive an approximate formula for the cumulative density of states,

$$N_{uc}(\omega) \approx 1 - \left(\frac{\gamma}{2\omega_g}\right)^{1/2} (\omega_{be} - \omega)^{1/2}, \tag{21}$$

which is of the general form expected at the band edge in one dimension. Taking $\omega \to 0$ in equation 20 gives

$$N_{uc}(\omega) \approx \omega/\omega_g \tag{22}$$

near the bottom of the band, which is the result we would expect from consideration of the mean electric and displacement fields when the wavelength is much larger than the period of the structure (*13*).

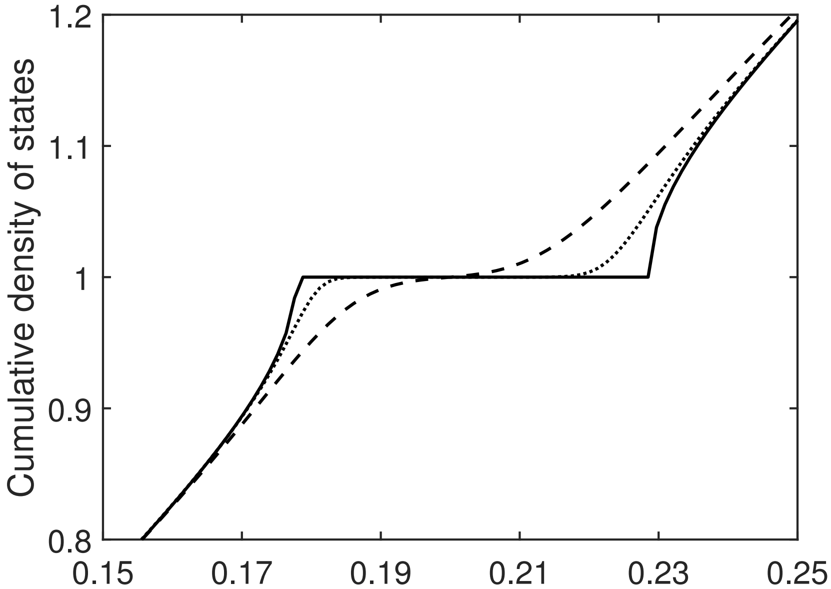

Figure 4. Solid curve: The cumulative density of states per unit cell versus normalized angular frequency $\omega a/2\pi c$ $(= \sigma)$ near the lowest bandgap of the photonic crystal described in the caption of figure 1. Solid curve: as given by equation 20 for the perfect crystal. Dotted curve: for a disordered crystal (see section 5) with $\Delta = 0.0266$. Dashed curve: for a disordered crystal with $\Delta = 0.1333$.

To gain a physical picture of the solutions to equation 15 we note that it can be considered to be the high friction limit (inertial effects neglected) of the equation of motion in ‘time’ [y] of a phase point at ‘position’ [ψ] under the action of a ‘force per unit mass’ resulting from a constant component [$2n_0\sigma - 1$] and a sinusoidal component [$(n_0\sigma\gamma/2)\sin\psi$]. That ‘force’ can be described by a tilted cosinusoidal potential in ψ-space.

It is interesting to note that equation 15 is very similar in form to equation 17 in (*2*) despite the refractive index profile of the photonic crystal considered being rather different. The crystal considered in that paper comprises alternate homogeneous layers of two different materials, but a common feature with the photonic crystal considered here is the equal thickness of the component layers resulting in an odd symmetry of the refractive index profile about the interlayer interface. With such structures the averaging procedure adopted to approximate equation 13 is generally expected to lead to similar results.

4. Reflectivity of the model one-dimensional photonic crystal

The wave admittance of a wave in the photonic crystal is $Y(x) = B(x)/\mu_0 E(x)$, where $B(x)$ is the magnetic induction. If we define a normalized wave admittance $\tilde{Y}(x)$ by dividing $Y(x)$ by the intrinsic admittance of free space, $(\mu_0 c)^{-1}$, then

$$\tilde{Y}(x) = \frac{cB(x)}{E(x)} = \frac{-i/k_0}{E(x)}\frac{dE(x)}{dx}, \tag{23}$$

which is also a logarithmic derivative of the electric field but, in contrast to the definition of $X(x)$ in equations 2, $E(x)$ is generally a complex quantity here.

The potential of the impedance/admittance concept to describe the optical properties of structures comprising discrete layers was recognized decades ago (see for example (*14*, *15*)) but the more flexible and powerful transfer matrix method (*16*) is now generally preferred. However, the admittance approach does have some virtue in describing systems where the dielectric properties vary continuously. For example, we can use $\tilde{Y}(x)$ to calculate the normal-incidence reflectivity of our model one-dimensional photonic crystal when it has finite extent. Consider a wave in a medium of refractive index n_i propagating in the x-direction and incident on the model photonic crystal and a transmitted wave emerging into a medium of refractive index n_t. The amplitude reflection coefficient r is given by

$$r = \frac{\tilde{Y}_{0i} - \tilde{Y}_{int}}{\tilde{Y}_{0i} + \tilde{Y}_{int}} = \frac{n_i - \tilde{Y}_{int}}{n_i + \tilde{Y}_{int}}, \tag{24}$$

where $\tilde{Y}_{0i}$ is the normalized intrinsic admittance of the medium of incidence and $\tilde{Y}_{int}$ is the normalized wave admittance at the interface of incidence and can be considered to be the normalized input admittance presented to the incident wave by the structure. The intrinsic impedance of the medium of incidence is simply n_i.

To calculate $\tilde{Y}_{int}$ we note that the wave admittance is continuous across any interfaces in the system including the one between the photonic structure and the external medium of transmission. Hence $\tilde{Y}_t = \tilde{Y}_{0t}$ where $\tilde{Y}_t$ is the normalized wave admittance at the interface with the transmission medium and $\tilde{Y}_{0t} = n_t$ is the normalized intrinsic admittance of the external transmission medium. With a knowledge of $\tilde{Y}_t$ and the dependence of the refractive index $n(x)$ on position x in the photonic structure, $\tilde{Y}_i$ and hence r in equation 24 may be obtained.

Comparing equations 2 and 23, it is apparent that the equation determining $\tilde{Y}(x)$ can be obtained by substituting $X = i\alpha\tilde{Y}$ into equation 4 to give

$$\frac{d\tilde{Y}(x)}{dx} = ik_0 \left(n(x)^2 - \tilde{Y}(x)^2 \right). \tag{25}$$

For the particular case of the model photonic structure with relative permittivity profile defined by equation 7,

$$\frac{d\tilde{Y}(y)}{dy} = i\sigma \left(n_0^2(1 + \gamma \sin y) - \tilde{Y}(y)^2 \right). \tag{26}$$

Note that while X defined in equation 1 is real and exhibits singularities that are the very essence of its usefulness, for the type of propagating wave problem considered here, $\tilde{Y}$ is generally complex and there are no divergences to complicate a numerical solution of equation 26.

For the purposes of illustration we consider the specific case where the photonic crystal has 10 unit cells, $n_0 = 2.5$, $\gamma = 0.5$ and $n_i = n_t = 1$. The existence of the photonic bandgap seen in the density of states calculations of section 3 is apparent in the reflectivity spectrum as the band where $|r|$ is very close to unity in figure 5, and can be attributed to the large magnitude of the normalized input admittance at the incident interface.

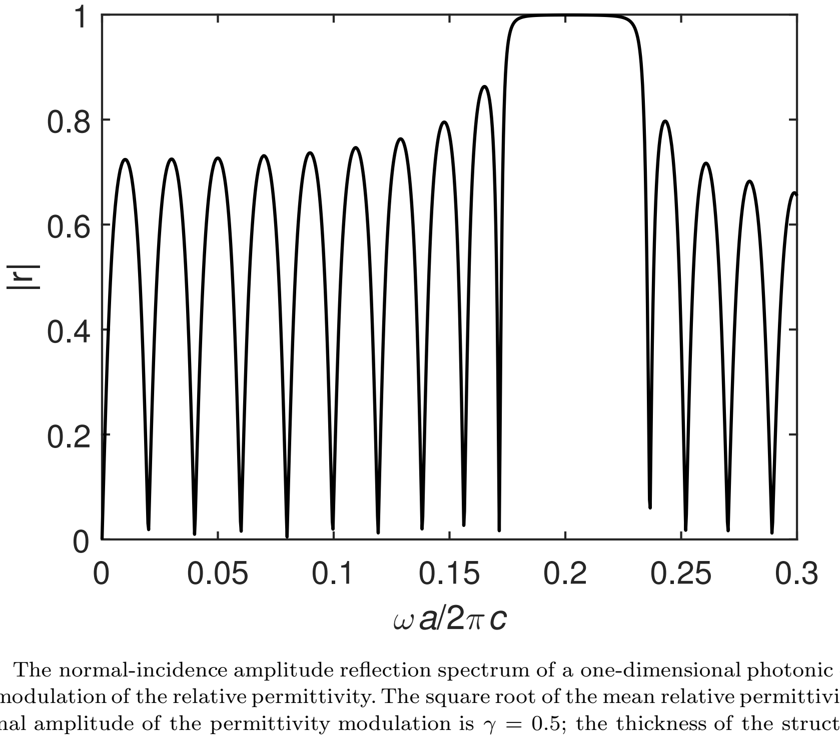

Figure 5. The normal-incidence amplitude reflection spectrum of a one-dimensional photonic crystal with a sinusoidal modulation of the relative permittivity. The square root of the mean relative permittivity is $n_0 = 2.5$; the fractional amplitude of the permittivity modulation is $\gamma = 0.5$; the thickness of the structure is 10 unit cells and the external medium is vacuum.

The admittance method does not provide a direct means of calculating the transmission spectrum and can only provide information on the magnitude of the transmission coefficient t in a lossless system, where the conservation of energy may be used to give

$$|t| = \sqrt{n_i(1 - |r|^2)/n_t}\,.$$

5. Using the phase formalism to calculate the cumulative density of states of a disordered photonic crystal

The cumulative density of states of a disordered photonic crystal may be calculated by using the same approach as for a perfect crystal when a suitable random component is included in the relative permittivity function, $n(x)^2$. For a sufficiently large sample, self-averaging means that the density of states is the same as the configuration-averaged density of states obtained by considering a large ensemble of systems. That correspondence facilitates an alternative method of calculation in some circumstances. Such an approach (*1*, *2*, *9*) is to obtain the distribution function of ψ for an ensemble of systems and then use that to calculate the mean value of $N_{uc}(\omega)$, as given in equation 14.

To consider the effect of disorder on our model crystal, we take the relative permittivity to be given by

$$n(y)^2 = n_0^2(1 + \gamma \sin y + \Gamma(y)), \tag{27}$$

where Γ describes a random modulation in addition to the periodic modulation considered hitherto. In (*1*, *2*) random fluctuations of the refractive index from layer to layer were considered, but here we consider a very different kind of disorder. We take the disorder in the relative permittivity to be on a much shorter length scale and described by a white noise autocorrelation function,

$$\langle \Gamma(y)\Gamma(y')\rangle = 2\Delta\delta(y - y'), \tag{28}$$

where $\delta(y - y')$ is a Dirac delta function. This model of disorder allows us to use directly some well-established theory of stochastic processes to derive an equation for the distribution function of ψ. However, as we are interested in the behaviour of ψ over many unit cells for the calculation of the density of states, there is scope for using this zero-correlation-length model more generally to describe various types of disorder on a range of length scales by suitable choice of the spectral power density.

In the presence of the disorder, equation 13 becomes

$$\frac{d\psi(y)}{dy} = 2n_0\sigma - 1 + n_0\sigma\left[\gamma \sin y + \Gamma(y)\right]\left[1 - \cos(y + \psi(y))\right], \tag{29}$$

which can be considered to be a Langevin equation (*17*) of the dynamical system described at the end of section 3 when there is a fluctuating 'force' $n_0\sigma\left[1 - \cos(y + \psi(y))\right]\Gamma(y)$. In contrast to the Langevin equation for the photonic structure considered in (*1*, *2*), the fluctuating 'force' $\Gamma(y)$ is multiplied by a y-dependent quantity and is therefore a case of what is called multiplicative noise in the literature. In the case of a perfect crystal ($\Gamma(y) = 0$), N_{uc} has been calculated using equation 14 as the 'mean velocity of ψ' plus unity. When there is randomness the 'velocity' can be calculated numerically for each system in an ensemble and then the ensemble average taken. However, further algebraic analysis is possible by deriving an equation for the distribution function of ψ and then using it to obtain the mean 'velocity' as done by (*1*, *2*). Such a Fokker-Planck equation corresponding to equation 29 can be derived following the general procedure described by Risken and Coffey et al (*9*, *17*), and is

$$\frac{\partial W(\psi,y)}{\partial y} = -\frac{\partial}{\partial\psi}D^{(1)}W(\psi,y) + \frac{\partial^2}{\partial\psi^2}D^{(2)}W(\psi,y) = -\frac{\partial S}{\partial\psi}, \tag{30}$$

where $W(\psi,y)$ is the distribution function of ψ and

$$\begin{aligned} D^{(1)} &= 2n_0\sigma - 1 + n_0\sigma\gamma\sin y\,[1-\cos(y+\psi)] + \frac{\Delta n_0^2\sigma^2}{2}\frac{\partial}{\partial y}\,[1-\cos(y+\psi)]^2\,, \\ D^{(2)} &= \Delta n_0^2\sigma^2\,[1-\cos(y+\psi)]^2\,. \end{aligned}$$

The second equality in equation 30 casts it in the form of a continuity equation with probability current S.

For the calculation of the cumulative density of states our interest is in solutions for the distribution function that are representative of the states in the bulk of a large structure. If the coefficients $D^{(1)}$ and $D^{(2)}$ were independent of y we would seek stationary solutions of equation 30 (that is solutions for which $\partial W(\psi,y)/\partial y = 0$ everywhere). However, since that is not the case, to make further algebraic progress we must approximate equation 30 while bearing in mind the type of solution required. In a similar spirit to our analysis in section 3, here we seek approximate solutions that are stationary in the sense that the net change in $W(\psi,y)$ across a photonic crystal unit cell is zero. Then integrating equation 30 over a unit cell while neglecting the y-variation of $W(\psi,y)$ gives

$$-\frac{\partial}{\partial\psi}\left(F+G\sin\psi\right)W + \Theta\frac{\partial^2 W}{\partial\psi^2} = -\frac{\partial S}{\partial\psi} = 0 \tag{31}$$

and hence

$$\Theta\frac{\partial W}{\partial\psi} = (F+G\sin\psi)W - S, \tag{32}$$

where $\Theta = 3n_0^2\sigma^2\Delta/2 = (3\Delta/8)(\omega/\omega_g)$ and F and G are as defined earlier. The probability current S is a constant by virtue of equation 31 and is proportional to the ensemble-averaged 'velocity', which we wish to obtain.

The problem is analogous to that of the high friction limit of Brownian motion of a particle in a tilted cosinusoidal potential, studies of which have been extensively reported in the literature. The solution of equation 32 has been described in some detail by Risken (*9*) and we closely follow that approach here. The general solution to equation 32 is

$$W(\psi) = \exp\left(-V(\psi)/\Theta\right)\left[N - \frac{S}{\Theta}\int_0^{\psi}\exp\left(V(\psi')/\Theta\right)d\psi'\right], \tag{33}$$

where $V(\psi) = G\cos\psi - F\psi$ and N is an arbitrary constant. However, we require the distribution function $W(\psi)$ to be bounded for all ψ and Risken shows that under those circumstances N must be given by

$$N = \frac{SH^{+}_{2\pi}}{\Theta\left(1-\exp(-2\pi F/\Theta)\right)}, \tag{34}$$

where

$$H^{+}_{2\pi} = \int_0^{2\pi} \exp\left(V(\psi')/\Theta\right) d\psi'. \tag{35}$$

Furthermore, $W(\psi)$ is then periodic with period 2π and it is appropriate to normalize it over one period:

$$\int_0^{2\pi} W(\psi)\, d\psi = 1. \tag{36}$$

As previously explained, the ensemble-averaged cumulative density of states is given by $\langle \psi(y_2) - \psi(y_1))/(y_2 - y_1)\rangle + 1$ where the angular brackets denote the ensemble-averaging. Using the stationary distribution function $W(\psi)$ we can write

$$\langle \psi(y_2) - \psi(y_1))/(y_2 - y_1)\rangle = \langle \partial\psi/\partial y\rangle = \int_0^{2\pi} W(\psi)\, \partial\psi/\partial y\, d\psi.$$

It follows from equations 29, 15, 32 and the periodicity of $W(\psi)$ that

$$\langle \partial\psi/\partial y\rangle = \langle F + G\sin\psi\rangle = \langle \Theta\partial W/\partial\psi + S\rangle = 2\pi S.$$

Therefore the calculation of $\langle \partial\psi/\partial y\rangle$ reduces to the determination of the current S. As is apparent from equations 33 and 34, an explicit expression for S follows from the normalization of W and the ensemble-averaged cumulative density of states per unit cell $\langle N_{uc}\rangle$ is given by

$$\langle N_{uc}\rangle = 1 + 2\pi S = 1 + \frac{2\pi\Theta\left(1-\exp(-2\pi F/\Theta)\right)}{H^{+}_{2\pi}H^{-}_{2\pi} - \left(1-\exp(-2\pi F/\Theta)\right) H^{+}_{\psi}H^{-}_{2\pi}}, \tag{37}$$

where

$$H^{-}_{\beta} = \int_0^{\beta} \exp\left(-V(\psi')/\Theta\right) d\psi'.$$

Figure 4 shows the cumulative density of states predicted by equation 37 for photonic crystals with two levels of disorder ($\Delta = 0.0266$ and $\Delta = 0.1333$) in comparison with the perfect crystal. The density of states per *unit angular frequency* per unit cell can be obtained by differentiating $\langle N_{uc}(\omega)\rangle$ with respect to ω, and inspection of the gradient of the curve for $\Delta = 0.0266$ shows there is significant encroachment by states into the bandgap of the perfect crystal. Nevertheless the cumulative density of states is constant (and hence the density of states per unit angular frequency is zero) throughout most of the bandgap. As expected, the band tailing increases with the level of disorder; it is markedly greater for the case of $\Delta = 0.1333$ illustrated and increasing the disorder further eventually obliterates the bandgap. However, it is apparent for the cases illustrated in figure 4 that the cumulative density of states remains unity at the centre of the gap. In fact equation 37 predicts that, whatever the level of disorder, $\langle N_{uc}(\omega_g)\rangle = 1$ because when $\omega \to \omega_g$, $F = (\omega - \omega_g)/\omega_g \to 0$, and

$$\langle N_{uc}\rangle \to 1 + F/H^{+}_{2\pi}H^{-}_{2\pi} \to 1 + F/\left[I_0((G/\Theta)\right]^2 ,$$

where I_0 is a modified Bessel function of zero order.

6. Conclusions

We have studied the properties of a phase formalism in the calculation of the cumulative density of states of one-dimensional photonic crystals. To simplify the analysis and provide a clear illustration of the properties, we have deliberately chosen a simple model of the photonic crystal. However, the results are of more general application and, in particular, it is apparent from the analysis that the theoretical framework will be similar for more practical structures that share the property of alternating dielectric layers of equal thickness and, with a little more analysis, for more general structures. The differential equation describing the phase variable has been solved numerically to show the spatial dependence of the phase in the first photonic bandgap, where its behaviour is not so intuitively predictable, as well as in the lowest allowed band. Also by making some straightforward approximations to the differential equation, it has been possible to derive a simple formula for the cumulative density of states. In addition it has been shown that related theory may be used in numerical calculations of the reflectivity of finite photonic crystals, and is an approach with some advantages over the popular transfer matrix method when the refractive index profile varies continuously.

In a disordered photonic crystal the phase becomes a stochastic variable. For certain models of disorder it is possible to derive a differential equation to describe the distribution function of the phase variable and then use the solution of that to obtain the ensemble-averaged cumulative density of states. In the case of the model crystal studied we have demonstrated that the problem can be reduced to one that is analogous to Brownian motion in a tilted-cosinusoidal potential. Using the theory, analytical and numerical results have been obtained to illustrate how increasing disorder causes increasing band-tailing in the first photonic bandgap.

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References

(1) Greshnov, A.A.; Kaliteevski, M.A.; Abram, R.A.; Brand, S.; Zegrya, G.G. Density of states of one-dimensional disorderd photonic crystals, *Phys. Solid State* **2007**, *49*, 1999.
(2) Greshnov, A.A.; Kaliteevski, M.A.; Abram, R.A.; Brand, S.; Zegrya, G.G. Density of states of 1D disorderd photonic crystals: analytical solution, *Sol. Stat. Comm* **2008**, *146*, 157.
(3) Courant, R.; Hilbert, D. *Methods of Mathematical Physics - Volume 1*; Wiley, 1953.

(4) James, H.M.; Ginzbarg, A.S. Band structure in disordered alloys and impurity semiconductors, *J. Phys. Chem.* **1953**, *57*, 840.

(5) Schmidt, H. Disordered one-dimensional crystals, *Phys. Rev.* **1957**, *105*, 425.

(6) Frisch, H.L.; Lloyd, S.P. Electron levels in a one-dimensional random lattice, *Phys. Rev.* **1960**, *120*, 1175.

(7) Halperin, B.I. Properties of a particle in a one-dimensional random potential, *Adv. Chem. Phys.* **1967**, *13*, 123.

(8) Lifshits, I.M.; Gredeskul, S.A.; Pastur, L.A. *Introduction to the Theory of Disordered Systems*, 3rd ed.; Wiley, 1988.

(9) Risken, H. *The Fokker-Planck Equation*, 2nd ed.; Springer, 1989.

(10) Greshnov, A.A.; Kaliteevski, M.A.; Abram, R.A. Analytical theory of light localization in one-dimensional disordered photonic crystals, *Sol. Stat. Comm* **2013**, *158*, 38.

(11) Kaliteevski, M.; Beggs, D.M.; Brand, S.; Abram, R.A.; Nikolaev, V.V. Statistics of the eigenmodes and optical properties of one-dimensional disordered photonic crystals, *Phys. Rev. E* **2006**, *73*, 056616.

(12) Gradshteyn, I.S.; Ryzhik, I.M. *Table of Integrals, Series and Products*, 7th ed.; Academic Press, 2007.

(13) Markos, P.; Soukoulis, C.M. *Wave Propagation*, 1st ed.; Princeton University Press, 2008.

(14) Schelkunoff, S.A. The impedance concept and its application to problems of reflection, refraction, shielding and power absorption, *Bell Syst Tech. J.* **1938**, *17*, 17.

(15) Kronig, R.; Blaisse, B.S.; Sande, J.J.V.D. Optical impedance and surface coating, *Appl. Sci. Res. B* **1947**, *1*, 63.

(16) Born, M.; Wolf, E. *Principles of Optics*, 6th ed.; Cambridge University Press, 1980.

(17) Coffey, W.T.; Kalmykov, Y.P.; Waldron, J.T. *The Langevin Equation*, 2nd ed.; World Scientific, 2004.