Long-wavelength behavior of two-dimensional photonic crystals

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We solve *analytically* the multiple-scattering equations for two-dimensional photonic crystals in the longwavelength limit. Different approximations of the electric and magnetic susceptibilities are presented from a unified pseudopotential point of view. The nature of the so-called plasmon-polariton bands is clarified. Its frequency as a function of the wire radius is discussed. The corresponding tunable "magnetic surface plasmon" band is pointed out.

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There has been much interest recently in two-dimensional (2D) photonic crystals consisting of arrays of metallic or dielectric cylinders (wires) in an insulating matrix or arrays of insulating cylinders in a metallic matrix. These include recent interest in left-handed materials [1] and in plasmonics [2]. A key issue is the effective susceptibilities $\langle \epsilon \rangle$ and $\langle \mu \rangle$ of the system. To design systems at different frequencies such as in the infrared range, it is useful to know their values for different system parameters. Numerical results are not always readily available because sometimes the bands are complex. The photonic bands in an array of cylinders can be understood entirely in terms of the scattering phase shift of the cylinders. In the pseudopotential idea in electronic structure calculation, a real potential is replaced by an effective one so that the same scattering of the electrons is produced. Similarly effective susceptibilities can be introduced so that the correct scattering effect for electromagnetic waves is produced. We examine this idea to derive effective susceptibilities for the cylinder [see Eqs. (8), (9), and (18)]. For metallic cylinders, the magnitude of the wave vector inside the metal is of the order of the inverse skin depth of the metal. When the skin depth is much less than the radius of the cylinder, we obtain a dielectric constant of a metallic form where the effective "plasma frequency" is given by

$$\omega_p^{\prime \, 2} = -\frac{2c^2}{R^2 \ln(\omega R/c)},\tag{1}$$

with R being the radius of the cylinder. While the original analysis [3] for the effective dielectric constant is carried out for a wire radius less than the skin depth of the metal, the experiments [4] for the left-handed materials are performed for wires with radii larger than the skin depth. Our result provides for an extension of the original analysis. For the dielectric constant of a composite, there is an additional factor of the volume fraction of the wires. Except for a different logarithmic correction, the other factors of our formula are the same as that of Pendry and co-workers, when the volume fraction factor is taken into account.

This also clarifies the issue of damping. For frequencies from 1 to 10 GHz, the imaginary part of the dielectric constant of most metals is about 1000 times larger than the real part. When the skin depth is much less than the wire radius, the loss in the metal is only restricted near the surfaces of the wires and the effective damping is reduced. Indeed, our dielectric constant depends only on the wavelength and the wire radius, with no damping. When the effective wavelength inside the cylinder is less than its radius, we recover recent effective-medium results by Wu *et al.* [5] and Hu *et al.* [6].

In this Rapid Communication we further calculate the photonic band structure of an array of cylinders of radius R in the long-wavelength limit when the separation between the wires a is less than the free-space wavelength $\lambda = 2\pi/k_0$. We solve analytically the multiple-scattering equations in the long-wavelength limit. We find that the scattering phase shifts for both the s wave (n=0 partial wave) and the p wave $(n = \pm 1 \text{ partial waves})$ are of the same order of magnitude. $(k_0 R)^2$, and need to be considered. These produced *two* photonic branches: an "acoustic" mode with a frequency proportional to the wave vector with an effective dielectric constant $\langle \epsilon \rangle$ [Eq. (27)] and a magnetic susceptibility $\langle \mu \rangle$ [Eq. (28)] and an "optic" mode with a gap. For negative dielectric constants and narrow cylinders, the "optic" mode corresponds to a flatband at frequencies close to the surface plasmon resonances, as has been previously discovered numerically. For negative magnetic susceptibilities, a "magnetic surface plasmon" band is found. For the acoustic mode, we found that $\langle \epsilon \rangle$ can be expressed as the arithmetic mean of that of the medium and an effective dielectric constant of the cylinder ϵ_c' . We now describe our result in detail.

We first describe our "pseudopotential" idea for the effective dielectric constant of the cylinder. As far as the electromagnetic (EM) field outside the cylinder is concerned, the effect of the cylinder is completely determined by the scattering phase shifts η_n for various angular momentum components *n*. They are given, for the *E* (TM) and *H* (TE) modes, respectively, by [7]

$$\tan \eta_n^E = \frac{k_i J_n'(x) J_n(y) - k_o \epsilon J_n(x) J_n'(y)}{k_i N_n'(x) J_n(y) - k_o \epsilon N_n(x) J_n'(y)},$$
(2)

$$\tan \eta_n^H = \frac{k_i J_n'(x) J_n(y) - k_o \mu J_n(x) J_n'(y)}{k_i N_n'(x) J_n(y) - k_o \mu N_n(x) J_n'(y)}.$$
(3)

The subscripts *i* and *o* refer to quantities inside and outside the cylinder, respectively. $k_j = k_0(\mu_j \epsilon_j)^{1/2}$ for j = o and *i*, $\epsilon = \epsilon_i / \epsilon_o$, $\mu = \mu_i / \mu_o$, and $x = k_o R$, $y = k_i R$. We first focus on the *s* wave with n=0. For $x=k_0 R \ll 1$, with $J_0(x)=1$, $J'_0(x)=-x/2$, $N_0(x)=(2/\pi)\ln x$, and $N'_0(x)=2/(\pi x)$, one has

$$\tan \eta_0^E \approx -\frac{\pi x^2}{4} \frac{1 + 2\epsilon J'/(yJ)}{1 - yJ' \ln x/(\mu J)},$$
 (4)

$$\tan \eta_0^H = -\frac{\pi x^2}{4} \frac{1 + 2\mu J'/(yJ)}{1 - yJ' \ln x/(\epsilon J)},$$
(5)

where $J=J_0(y)$ and $J'=J'_0(y)$. If $y=k_iR$ is also small, we have

$$\tan \eta_0^E \approx -\frac{\pi}{4} x^2 [1 - \epsilon], \quad \tan \eta_0^H \approx -\frac{\pi}{4} x^2 [1 - \mu].$$
 (6)

As is expected, when $\epsilon = 1$, there is no scattering and $\tan \eta_0^E = 0$. When $k_i R$ is not small, one can *define* effective susceptibilities so that the same phase shift is produced:

$$\tan \eta_0^E \approx -\frac{\pi}{4} x^2 [1 - \epsilon_E'], \quad \tan \eta_0^H \approx -\frac{\pi}{4} x^2 [1 - \mu_H'].$$
(7)

This is the "pseudopotential" idea that we mentioned. From Eq. (7) we obtain

$$\epsilon'_E = -\frac{\epsilon J'}{yJ} \frac{2 + x^2 \ln x}{1 - yJ' \ln x/(\mu J)},\tag{8}$$

$$\mu'_{H} = -\frac{\mu J'}{yJ} \frac{2 + x^{2} \ln x}{1 - yJ' \ln x/(\epsilon J)},$$
(9)

for the effective dielectric constant and magnetic susceptibility. For metallic cylinders, the magnitude of the wave vector inside the metal, k_i , is of the order of the inverse skin depth of the metal. When the skin depth is much less than the radius of the cylinder, $k_i R \ge 1$, the second term in the denominator is larger than the first term; assuming the outer region to be air with $\epsilon_o = \mu_o = 1$, we obtain an effective dielectric constant of a metallic form

$$\boldsymbol{\epsilon}_E' = 1 - \frac{\omega_p'^2}{\omega^2},\tag{10}$$

where ω'_{P} is given in Eq. (1).

Equation (8) encompasses other recent results for dielectric rods. If the second term of the denominator is much smaller than the first term, we recover recent results in [5,6]: namely,

$$\epsilon'_E \approx -\frac{2J'\epsilon}{Jk_i R}.$$
(11)

This pseudopotential idea is also implicit in recent results using cylinders with a high dielectric constant ferroelectric [8]. Equation (8) extends these results to more general regions of the parameter space.

For μ'_{H} , the second term in the denominator is of the order of $(\mu_i/\epsilon_i)^{1/2}x$ and is usually smaller than the first term. We obtain

$$\mu'_H \approx -\frac{2J'\mu}{Jk_i R}.$$
 (12)

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We next investigate the phase shifts for the higher-order partial waves. In the limit $x=k_o R \ll 1$,

$$\tan \eta_n^E = -\frac{\pi (x/2)^{2n}}{(n-1)!n!} \frac{\mu_o - n\mu_i J_{n'}(yJ'_n)}{\mu_o + n\mu_i J_{n'}(yJ'_n)},$$
(13)

$$\tan \eta_n^H = -\frac{\pi (x/2)^{2n}}{(n-1)!n!} \frac{\epsilon_o - n\epsilon_i J_n/(yJ'_n)}{\epsilon_o + n\epsilon_i J_n/(yJ'_n)}.$$
 (14)

Here $J_n = J_n(k_i R)$ and $J'_n = J'_n(k_i R)$. When $|k_i R| \le 1$,

$$\tan \eta_n^E = -\frac{\pi (x/2)^{2n}}{(n-1)!n!} \frac{\mu_o - \mu_i}{\mu_o + \mu_i},$$
$$\tan \eta_n^H = -\frac{\pi (x/2)^{2n}}{(n-1)!n!} \frac{\epsilon_o - \epsilon_i}{\epsilon_o + \epsilon_i}.$$
(15)

There is recently much interest in "plasmonics" when the frequency is close to the interface plasmon frequency so that $\epsilon = -1$. At this frequency $\eta_n^H = \pi/2$. Scattering resonances are exhibited for the TE modes for all $n \neq 0$. For n=1 the requirement that the same scattering phase shift should be obtained even when $k_i R$ is not small provides for the equations determining the effective susceptibilities:

$$\tan \eta_1^E = -\frac{\pi x^2}{4} \frac{\mu_o - \mu'_E}{\mu_o + \mu'_E},$$
 (16)

$$\tan \eta_1^H = -\frac{\pi x^2}{4} \frac{\epsilon_o - \epsilon'_H}{\epsilon_o + \epsilon'_H}.$$
 (17)

From these we obtain the effective susceptibilities

$$\mu'_E = \frac{\mu_i J_1}{J_1' k_i R}, \quad \epsilon'_H = \frac{\epsilon_i J_1}{J_1' k_i R}.$$
 (18)

Similar equations have also been obtained in [5,6] from a coherent potential approximation. The results here provide a different interpretation of their results. With the current view, "plasmonics" phenomena can also be manifested for nonmetallic rods if $\epsilon'_H + \epsilon_o = 1$ and the same scattering phase shift is produced.

We next examine a possible generalization of the pseudopotential idea to scattering units other than cylinders (or spheres). The scattering information is contained in the Tmatrix, which, in the angular momentum basis, can be written as $T = \Sigma |n\rangle T_{nm} \langle m|$. In the long-wavelength limit, the Tmatrix becomes $T = \Sigma |n\rangle T_{nm}^{0}(\epsilon, \mu) \langle m|$. Effective tensors ϵ and μ may be obtained if the equations $T_{nm} = T_{nm}^{0}(\epsilon, \mu)$ can be solved.

We now turn to the photonic bands.

We employ the multiple-scattering method, also known as the Korringa-Kohn-Rostoker (KKR) technique [9]. Denote the amplitude of the partial scattered wave with angular momentum *n* by a_n . The sum of the scattered waves from all the *other* sites becomes an incoming wave at the origin with the amplitude $p_n = \sum_n a_{n'} S(n-n')$, where

$$S(m) = \sum_{R \neq 0} e^{ik \cdot R} H_m(k_o R) e^{im\phi_R}.$$
 (19)

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Note that *S* does *not* include the wave from the origin; thus, the sum does not include the term at R=0. The outgoing scattered wave at the origin is related to the incoming wave by the *t* matrix: $a_n = t_n p_n$. With the definition of p_n , we arrive at the equation det $[S(n-n') - \delta_{nn'}/t_n]=0$. Here $\delta_{nn'}$ denotes the Kronecker δ symbol. Since the *t* matrix is related to the phase shift by $t_n = \tan \eta_n / (\tan \eta_n + i)$, we obtain the KKR equation

$$\det[A(n-n') - \delta_{nn'} \cot \eta_n] = 0.$$
⁽²⁰⁾

Here the structure factor $A(n) = [S(n) - \delta_{n0}]/i$.

In the long-wavelength limit, one can approximate the sum for S by an integral, which can then be analytically evaluated [10]. The structure factor becomes

$$A(n) \approx \frac{4i^{n}e^{in\phi_{k}}k^{n}}{k_{n}^{n}(k^{2}-k_{n}^{2})a^{2}}.$$
(21)

As is discussed above, if the wavelength outside the cylinder is long and $k_o R \ll 1$, tan $\eta_n \propto (k_o R)^{2n}$ for $n \neq 0$, tan $\eta_0 \propto (k_o R)^2$. The phase shifts for the *s* and *p* waves are of the same order of magnitude, $(k_o R)^2$, and need to be considered. When only the *s*- and *p*-wave components are kept, the KKR equation reduces to

$$HE = 0, \qquad (22)$$

where

$$\boldsymbol{H} = \begin{bmatrix} A(0) - \cot \eta_1 & A(1) & A(2) \\ A(1)^* & A(0) - \cot \eta_0 & A(1) \\ A(2)^* & A(1)^* & A(0) - \cot \eta_1 \end{bmatrix}.$$
 (23)

There are two classes of solutions, with either $E_1 = E_{-1}^* = |E_1|e^{i\phi_k}$ and $E_0 = E_0^*$ or $E_1 = -E_{-1}^* = i|E_1|e^{i\phi_k}$ and $E_0 = 0$. We get two possible eigenvalue equations. The first one is given by

$$[A(0) - \cot \eta_1 + |A(2)|][A(0) - \cot \eta_0] - 2|A(1)|^2 = 0.$$
 (24)

For the second case, we get

$$A(0) - \cot \eta_1 + |A(2)| = 0.$$
(25)

As we show below, the first mode corresponds to an "acoustic" branch with a frequency proportional to the wave vector, enabling an effective-medium description for the system; the second mode corresponds to a band with a gap. For negative susceptibilities, this corresponds to a flatband at frequencies close to the surface plasmon resonances, as has been previously found numerically [2].

We discuss the acoustic branch first. Substituting in the expressions for the phase shifts and the structure factor into Eq. (24) and after some algebra [11], we obtain

$$k^2 = k_0^2 \langle \epsilon \rangle \langle \mu \rangle, \qquad (26)$$

where

$$\langle \boldsymbol{\epsilon} \rangle = (1 - f)\boldsymbol{\epsilon}_o + f\boldsymbol{\epsilon}_i', \qquad (27)$$

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$$\langle \mu \rangle = \mu_o \frac{\mu_i'(1+f) + \mu_o(1-f)}{\mu_i'(1-f) + \mu_o(1+f)},$$
(28)

with ϵ'_i and μ'_i denoting the effective susceptibilities of the cylinders.

In the static (zero-wave-vector and -frequency) limit, for the case with the *E* field along the axis, Eq. (27) reduces to $\langle \epsilon \rangle = (1-f)\epsilon_o + f\epsilon_i$, implying that the average dielectric constant is just the arithmetic mean of the dielectric constants of the components, as is well known [12].

In multilayer systems, a similar result is obtained [13]. In that case the effective μ is the harmonic mean of the components, while the effective dielectric constant is still the arithmetic mean of that of its components.

We next discuss the "optic" mode. Substituting in the expressions for the phase shifts and the structure factor A(n), the equation for the second optic mode becomes

$$\frac{2(k_o a)^2}{\pi} \ln \frac{k_o a}{2\sqrt{\pi}} = 4 - 4f^{-1}\frac{\mu_o + \mu'_E}{\mu'_E - \mu_o} + O(k^2)$$
(29)

for the E mode and

$$\frac{2(k_oa)^2}{\pi}\ln\frac{k_oa}{2\sqrt{\pi}} = 4 - 4f^{-1}\frac{\epsilon_o + \epsilon'_H}{\epsilon'_H - \epsilon_o} + O(k^2)$$
(30)

for the *H* mode. When *k* approaches zero, k_o is not zero. Let us illustrate the physics by looking at the *H* mode. The limit of small *f* is particularly interesting. In that limit, the frequency is determined by the condition that $\epsilon_o + \epsilon'_H = 0$, where ϵ'_H is given in Eq. (18).

For metallic cylinders with their radii less than the skin depths, $k_i R \ll 1$, $\epsilon'_H = \epsilon_i = 1 - \omega_p^2 / \omega^2$, where ω_p is the plasma frequency. $\epsilon_o + \epsilon_i = 0$ when ω is equal to the interface plasmon resonance, $\omega_{sp} = \omega_p / (1 + \epsilon_o)^{1/2}$. For small k, from the above equation, we see that $\omega(k) = \omega(k=0) + O(fk)$. If f is small, the dispersion is weak and the bands are flat. This flatband has been observed numerically previously [2]. The present calculation provides for a more direct analytic demonstration of this result. If $k_i R$ is not small, Eq. (18) suggests that even with insulating cylinders, flat "plasmonic" photonic bands can still be obtained if the following condition is satisfied:

$$\frac{\epsilon_i J_1}{J_1' k_i R} = -\epsilon_o. \tag{31}$$

Let us next look at the *E* mode; the condition becomes $\mu'_E/\mu_o = -1$. We call this the "magnetic surface plasmon" mode. Although a lot of interest in plasmonics has been focused on the condition $\epsilon'_H/\epsilon_o = -1$, the counterpart condition on μ has not been much discussed.

There is another way of thinking of this type of solutions. As can be seen from Eqs. (2) and (3), when the susceptibilities of the metal are negative, $\epsilon_o + \epsilon_m$ can become zero and tan $\eta = \infty$. The scattering can go through resonances due to the interface plasmon. This can lead to flat photonic bands, as has been observed in previous numerical calculations. In general, the more rapidly varying the phase shift, the flatter the band.

Pokrovsky and Efros [14] have recently investigated the propagation of EM waves in a periodic array of metallic cylinders (wires) in the limit $\kappa R \ge 1$. Our conclusion differs from theirs. In their work, an expression similar to our S(0) also appears. However, in their expression, the sum is over *all* R whereas the R=0 term is excluded in ours.

In conclusion, in this Rapid Communication we use a pseudopotential idea to derive effective susceptibilities of cylinders so as to mimic the scattering phase shifts of the system. We calculate analytically the long-wavelength limit photonic band dispersion in a 2D photonic crystal and explicitly demonstrate the flat "surface plasmon" photonic bands with small group velocity v_g , which are implicitly exploited in the study of plasmonics. The spatial extent of a wave packet Δx is of the order of $v_g/\Delta \omega$. For subwavelength localization $\Delta x \ll \lambda$ where λ is the wavelength. We thus obtain the condition $\Delta \omega \gg v_g/\lambda$. Because v_g is small, the spread

in frequency $\Delta \omega$ remains small. The corresponding *magnetic* surface plasmon bands are demonstrated. This has not been much discussed before, but can be used in *tunable* subwavelength microwave transmission.

At the surface plasmon frequency, the phase shift is equal to $\pi/2$ in the limit when the cylinder radius is small. Our pseudopotential idea suggests that "plasmonics" effect need not be restricted to metallic systems at the surface plasmon frequency. Other systems with the same resonance phase shift will lead to similar photonic bands to provide subwavelength transmission and thus can serve as alternative candidates.

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- [10] We change the variable R to $x=k_oR$ and get

$$S(0) = \sum_{x \neq 0} (\Delta x)^2 e^{ik \cdot x/k_o} H_0(x) / (k_o a)^2.$$

In the long-wavelength limit, Δx becomes small. We approximate this sum by an integral and get

$$S(0) \approx \int_{x_i}^{\infty} d^2 x \; e^{ik \cdot x/k_o} H_0(x)/(k_o a)^2.$$

We pick the lower limit so that the empty area remains the same $[\pi x_i^2 = (k_o a)^2]$. Since $e^{ia \cos(\theta)} = \sum_m i^m J_m(a)e^{im\theta}$, only the m=0 term remains in the integral. The radial integral can be easily done. [We assume that k_0 has a small imaginary part so that the upper-limit contribution can be set to zero.] We get $|S(0) \approx -2\pi x[[kJ'_0(x_k)H_0(x) - k_oJ_0(x_k)H'_0(x)]/[k_oa^2(k^2 - k_o^2)]]|_{x_i}$. Using the small argument expansions for the Bessel and Hankel functions in the limit $x \ll 1$, we obtain $S(0) \approx 1 + [4i[k_o^2 - (x_i^2/2)(k_o^2 - k^2)\ln(x_i/2)]/(k_oa^2(k^2 - k_o^2)])$,

$$A(0) \approx \frac{2[2\pi k_o^2 - (k_o a)^2 (k_o^2 - k^2) \ln(k_o a/2\sqrt{\pi})]}{\pi (k_o a)^2 (k^2 - k_o^2)}$$

with $x_k = kx/k_o$. For $n \neq 0$, in the limit $k_0 R \ll 1$,

$$S(n) \approx -2\pi i^{n} e^{in\phi_{k}} \frac{kJ'_{n}(x_{k})H_{n}(x) - k_{o}J_{n}(x_{k})H'_{n}(x)}{k_{o}a^{2}(k^{2} - k_{o}^{2})} \bigg|_{x_{i}}.$$

The dominant contribution in the long-wavelength limit is obtained by replacing H_n by iN_n , so

$$A(n) \approx \frac{4i^{n}e^{in\phi_{k}}k^{n}[1+O(k_{o}^{2}a^{2})]}{k_{o}^{n}(k_{o}a)^{2}(k^{2}/k_{o}^{2}-1)}$$

Define $u = k_o^2/(k^2 - k_o^2)$; then, $A(0) \approx 4u/(k_o a)^2$, [11] $\exp(-in\phi)A(n) \approx \alpha_n A(0)$, with $\alpha_n = (ik/k_o)^n$. Noting that the phase shifts are $\tan \eta_0 \approx \pi (k_o R)^2/(4c_0)$ and $\tan \eta_1$ $\approx \pi (k_o R)^2/(4c_1)$, where $c_0 \approx -\epsilon_o/(\epsilon_o - \epsilon_c)$ and c_1^{-1} $\approx -(\mu_o - \mu_c)/(\mu_o + \mu_c)$, with ϵ_c and μ_c being the effective susceptibilities of cylinder, we have

$$u^{2}\left[1+|\alpha_{2}|-2|\alpha_{1}|^{2}\right]-\frac{u}{f}\left[c_{1}+(1+|\alpha_{2}|)c_{0}\right]+\frac{c_{1}c_{0}}{f^{2}}=0.$$

 $f = \pi R^2 / a^2$ is the volume fraction of the cylinders. Now

We thus get $u[1 + |\alpha_2| - 2|\alpha_1|^2] = -1.$

$$uf[-c_1 - f - (1 - \alpha_2)c_0] + c_1c_0 = 0.$$

This can be written as

$$[-c_1 - f - (1 + k^2/k_o^2)c_0]f = -(k^2/k_o^2 - 1)c_1c_0.$$

Inserting the definitions of c_0 and c_1 yields

$$\frac{k^2}{k_o^2} = \frac{[\mu_c + \mu_o - f(\mu_o - \mu_c)][\epsilon_o - f(\epsilon_o - \epsilon_c)]}{[\mu_c + \mu_o + f(\mu_o - \mu_c)]\epsilon_o}$$

This is Eqs. (27) and (28).

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