Appendix. Scattering Matrix Method: 
Determination of the Field for a Finite Two-Dimensional Crystal formed by Dielectric Rods

This appendix will be devoted to a more detailed exposition than was possible in 
Section 3 of Chapter 2 of the scattering matrix method, also referred to as the 
multipole method or as the modal method. We shall more specifically consider the 
problem of the determination of the field in two-dimensional photonic crystals 
formed by an array of dielectric rods in the air.

A.1 Incident Field

In the coordinate system represented in Fig. A.1, the incident field illuminating the 
array of rods can be written as follows:

\[ E_z^i = \exp\left(ik_0n_{\text{ext}}(x\sin\Theta^{\text{inc}} - y\cos\Theta^{\text{inc}})\right) \]  

(A.1a)

A.2 Field inside the Rods

Inside an arbitrary dielectric rod with a permittivity \( \varepsilon_{r,\text{int}} \), the total field satisfies the 
following equation:

\[ \nabla^2 E_z + k_0^2 \varepsilon_{r,\text{int}} E_z = 0 \] 

(A.2)

We shall use a system of local polar coordinates \((r, \theta_j)\) with an origin located at 
the centre of the \( j \)th rod. For a fixed value of \( r_j \), the field is a periodic function of \( \theta_j \) 
with a period \( 2\pi \), and it can therefore be written in the form of a Fourier series:
We shall use the expression in polar coordinates of the scalar Laplacian:

\[ \nabla^2 V = \frac{\partial^2 V}{\partial r_j^2} + \frac{1}{r_j} \frac{\partial V}{\partial r_j} + \frac{1}{r_j^2} \frac{\partial^2 V}{\partial \theta_j^2} \]  

(A.4)

Let us now introduce the expression of the field given by Eq. A.3 in Eq. A.4. A straightforward calculation demonstrates that the Fourier coefficients satisfy the following equation:
A.2 Field inside the Rods

Assuming that \( r_j' = k r_{int} r_j \) and after proceeding to some simplifications, this equation becomes:

$$\forall m, \quad \frac{d^2 E_{z,m}}{dr_j^2} + \frac{1}{r_j} \frac{\partial E_{z,m}}{\partial r_j} + \left( k_0^2 \varepsilon_{r,\text{int}} - \frac{m^2}{r_j^2} \right) E_{z,m} = 0$$ (A.5)

We are therefore led back to Bessel’s equation. The general solution of this equation is given by:

$$E_{z,m} = c_{j,m} J_m \left( r_j \right) + d_{j,m} Y_m \left( r_j \right)$$

where \( J_m \) and \( Y_m \) are Bessel functions of the \( m^{th} \) order of the first and second kinds respectively (Abramovitz 1970).

The right-hand side of Eq. A.7 can also be written in the following form:

$$E_{z,m} = \left( c_{j,m} + i d_{j,m} \right) J_m \left( k r_{int} r_j \right) - i d_{j,m} \left( J_m \left( k r_{int} r_j \right) + i Y_m \left( k r_{int} r_j \right) \right)$$ (A.9)

Let us here remind ourselves that the definition of the Hankel function of \( m^{th} \) order of the first kind is:

$$H^{(1)}_m (u) = J_m (u) + i Y_m (u)$$ (A.9)

It thus turns out that Eq. A.8 can be re-written in the form:

$$E_{z,m} = c_{j,m} J_m \left( k r_{int} r_j \right) + d_{j,m} H^{(1)}_m \left( k r_{int} r_j \right)$$ (A.10)

where the coefficients \( c_{j,m} \) and \( d_{j,m} \) can be easily deduced from \( c'_{j,m} \) and \( d'_{j,m} \).

It shall be later demonstrated that this new expression of the field is the most adequate for a physical interpretation of the two terms appearing in its right-hand side. Introducing this expression for \( E_{z,m} \) in Eq. A.3, we arrive at an expression of the total field in the rod in terms of a Fourier-Bessel expansion:
Appendix. Scattering Matrix Method: Determination of the Field

\[ E_z(r_j, \theta_j) = \sum_{m = -\infty, +\infty} \left[ c_{j,m} J_m(k_0 n_{im} r_j) + d_{j,m} H_m^{(1)}(k_0 n_{im} r_j) \right] \exp(\imath m \theta_j) \quad (A.11) \]

It can be noted that in the specific case of the field inside the rods, all coefficients \( d_{j,m} \) become zero; indeed, the Hankel function \( H_m^{(1)}(s) \) presents a singularity at \( s = 0 \). Since the field cannot be singular, the corresponding terms have to be removed from the expression of the field, and therefore, for \( r_j < R \):

\[ E_z(r_j, \theta_j) = \sum_{m = -\infty, +\infty} c_{j,m} J_m(k_0 n_{im} r_j) \exp(\imath m \theta_j) \quad (A.12) \]

The determination of the field inside the rods thus reduces to the calculation of the coefficients \( c_{j,m} \) of the Fourier-Bessel expansion given in the right-hand side of Eq. A.12.

A.3 Field in the Vicinity of a Rod

The calculations which have led to the expression of the field inside the rods can be reproduced almost identically for the regions outside the rods.

Thus, the field outside the rods can be shown to satisfy the following Helmholtz equation:

\[ \nabla^2 E_z + k_0^2 \varepsilon_{r,ext} E_z = 0 \quad (A.13) \]

Let us now consider the circular region surrounding the \( j^{th} \) rod and extending to the nearest point of the immediately neighbouring rod. This region is represented by the light grey area in Fig 2.10 in Chapter 2. In this region the value of the refractive index is constant and equal to \( n_{ext} \). Using the same coordinate system and the same mathematical development than in the preceding section, it can be demonstrated that the field in this region assumes the form of a Fourier-Bessel series similar to the series given in Eq. A.11:

\[ E_z(r_j, \theta_j) = \sum_{m = -\infty, +\infty} a_{j,m} J_m(k_0 n_{ext} r_j) \exp(\imath m \theta_j) \]

\[ + \sum_{m = -\infty, +\infty} b_{j,m} H_m^{(1)}(k_0 n_{ext} r_j) \exp(\imath m \theta_j) \quad (A.14) \]

In this case however, it is no longer possible to demonstrate that the coefficients \( b_{j,m} \) are zero. Indeed, no physical argument prevents here the field from being singular at the origin, since this origin does not belong to the ring itself.
Nevertheless, the two terms appearing in the right-hand side of Eq. A.14 can be given a physical interpretation from the properties of Bessel functions. The field in the ring can indeed be decomposed into three different components:

- the incident plane wave, i.e. the source, given by Eq. A1,
- the field scattered by the $j^{th}$ rod. From the radiation condition at infinity, this field must propagate away from this rod,
- the fields scattered by the all other rods in the direction of the $j^{th}$ rod. These fields behaves with respect to this rod as an incident field. Accordingly, the total incident field at the $j^{th}$ rod is formed by these fields and by the incident plane wave, i.e. the source term.

In order to identify each physical component in Eq. A.14, it might be first noted that the total incident field at the $j^{th}$ rod is necessarily generated by sources located outside this rod. This field must therefore satisfy a Helmholtz equation inside this rod without presenting any singularity. This property allows us to conclude that the total incident field is contained in the first sum of Eq. A.14, and therefore that the second sum represents the field scattered by the $j^{th}$ rod. The only remaining question is whether this second sum represents the totality or only a part of the field scattered by the $j^{th}$ rod. In the first case, the first sum would represent the total incident field on this rod, whereas in the second case it would also contain a part of the field scattered by the $j^{th}$ rod complementary to the second sum. This question can be answered by observing that from causality the field scattered by the $j^{th}$ rod must propagate away from this rod. It can be demonstrated that the only Fourier-Bessel functions satisfying this condition are the Hankel functions of the first kind. For instance, apart from a multiplying factor, the Hankel function of zeroth order of the first kind is but the Green’s function solution for the Helmholtz equation in an homogeneous space with permittivity $\varepsilon_{r,\text{ext}}$ under the assumption of a radiation condition at infinity:

$$
\nabla^2 \left[ -\frac{i}{4} H_0^{(1)}(k_0 n_{\text{ext}} r_j) \right] + k_0^2 \varepsilon_{r,\text{ext}} \left[ -\frac{i}{4} H_0^{(1)}(k_0 n_{\text{ext}} r_j) \right] = \delta(x) \delta(y) \quad (A.15)
$$

From a physical point of view, the Green’s function thus defined represents the field that would be generated by an infinitely thin linear source located along the $z$ axis, i.e. parallel to the rods, the space being assumed to be homogeneous and with a permittivity $\varepsilon_{r,\text{ext}}$. In order to verify that Hankel functions of the first kind satisfy the radiation condition at infinity for any order, it suffices to consider their asymptotic expression at infinity (Abramovitz 1970):

$$
H_m^{(1)}(k_0 n_{\text{ext}} r_j) \approx \frac{2}{\pi k_0 n_{\text{ext}} r_j} \exp \left[ i \left( k_0 n_{\text{ext}} r_j - m \frac{\pi}{2} - \frac{\pi}{4} \right) \right] \quad (A.16)
$$
The second sum in Eq. A.14 represents a field scattered by the \( j^\text{th} \) rod. On the contrary, an arbitrary term of the first sum cannot represent a scattered field since, from Eq. A.9, \( J_m(s) \) can be written in the form:

\[
J_m(s) = \widetilde{H}_m^{(1)}(s) + \widetilde{H}_m^{(1)}(s)
\] (A.17)

where \( \widetilde{H}_m^{(1)}(s) \) denotes the complex conjugate of \( H_m^{(1)}(s) \). It is quite apparent from Eq. A.16 that \( \widetilde{H}_m^{(1)}(s) \) does not satisfy the radiation condition. This definitely demonstrates that the first sum in Eq. A.14 represents the total incident field striking the \( j^\text{th} \) rod and the second sum the field scattered by the \( j^\text{th} \) rod.

Let us now proceed to the determination of the contribution of the incident source field to the first sum. This field is given by Eq. A.1a, and at any arbitrary point \( P \) of space (Fig. A.1), it can be written in the form:

\[
E^I(P) = \exp(ik.OP)
\] (A.1b)

where \( (k_0n_{\text{ext}} \sin \Theta^{\text{inc}}, -k_0n_{\text{ext}} \cos \Theta^{\text{inc}}) \) are the coordinates of the incident wave vector \( k \). Writing vector \( OP \) as the sum of vectors \( O_jP \) and \( O_jO \), we arrive at the following equation:

\[
E^I(P) = \exp(ik(O_j + O_jP))
\] (A.18)

\[
= \exp\left[ik_0n_{\text{ext}}r_j^j \sin(\Theta^{\text{inc}} - \theta_j^j)\right] \exp\left[ik_0n_{\text{ext}}r_j^j(P) \sin(\Theta^{\text{inc}} - \theta_j(P))\right]
\]

where \( r_j^j, \theta_j^j \) denote the polar coordinates of the origin \( O_j \) of the local coordinate system in the general \( xy \) system represented in Fig. A.1. Let us now use the following formula, given in (Abramovitz 1970):

\[
\exp(i\xi \sin(u)) = \sum_{m=-\infty}^{\infty} J_m(\xi) \exp(imu)
\] (A.19)

The application of Eq. A.19 leads to the following expression for \( E^I(P) \):

\[
E^I(P) = \exp\left[ik_0n_{\text{ext}}r_j^j \sin(\Theta^{\text{inc}} - \theta_j^j)\right] \times
\sum_{m=-\infty, +\infty} \exp(im\Theta^{\text{inc}})J_m(k_0n_{\text{ext}}r_j^j(P)) \exp(-im\theta_j(P))
\] (A.20a)
Since \( J_m(s) = (-1)^m J_m(s) \), \( m \) can be replaced by \(-m\) in Eq. A.20a. This shall simplify the comparison with the terms in Eq. A.14:

\[
E^i(P) = \exp \left[ ik_0 n_{\text{ext}} r^j \sin(\Theta^{\text{inc}} - \theta^j) \right] \sum_{m=-\infty, \pm \infty} (-1)^m \exp(-im\Theta^{\text{inc}}) J_m(k_0 n_{\text{ext}} r^j(P)) \exp(im\theta^j(P)) \tag{A.20b}
\]

Eqs. A.20a and A.20b give the development of the incident source field into Fourier-Bessel series in the coordinate system associated with the \( j^\text{th} \) rod. Going back to Eq. A.14, it is now possible to distinguish the coefficients of the Fourier-Bessel series associated with the source field from the coefficients associated with the field scattered by the other rods. These two sets of coefficients will be denoted by \( a_{j,m}^{\text{source}} \) and \( a_{j,m}^{\text{rods}} \) respectively, and their sum is equal to \( a_{j,m} \). From Eq. A.20b, \( a_{j,m}^{\text{source}} \) can be identified with the following expression:

\[
a_{j,m}^{\text{source}} = (-1)^m \exp \left( ik_0 n_{\text{ext}} r^j \sin(\Theta^{\text{inc}} - \theta^j) - im\Theta^{\text{inc}} \right) \tag{A.21}
\]

The three components of the field in the ring surrounding the \( j^\text{th} \) rod can therefore be expressed respectively as follows:

- the source term is:

\[
E_{c,j}^{\text{source}}(r_j, \theta_j) = \sum_{m=-\infty, \pm \infty} a_{j,m}^{\text{source}} J_m(k_0 n_{\text{ext}} r_j) \exp(im\theta_j) \tag{A.22}
\]

- the field scattered by the other rods in the direction of the \( j^\text{th} \) rod is:

\[
E_{c,j}^{\text{rods}}(r_j, \theta_j) = \sum_{m=-\infty, \pm \infty} a_{j,m}^{\text{rods}} J_m(k_0 n_{\text{ext}} r_j) \exp(im\theta_j) \tag{A.23}
\]

- the field scattered by the \( j^\text{th} \) rod is:

\[
E_{c,j}^{d}(r_j, \theta_j) = \sum_{m=-\infty, \pm \infty} b_{j,m} H_{m}^{(1)}(k_0 n_{\text{ext}} r_j) \exp(im\theta_j) \tag{A.24}
\]

It has been demonstrated that the total field in the ring can be expressed in terms of three series of coefficients: \( a_{j,m}^{\text{source}} \), \( a_{j,m}^{\text{rods}} \) and \( b_{j,m} \), from which only the
first is known. Before proceeding to the calculation of these components, an observation should be made on Eq. A.24. The expression given by this equation for the field scattered by the \( j^\text{th} \) rod in the circular region surrounding it (see Figure 2.10 in Section 3 of Chapter 2) extends actually to the whole space surrounding this rod. While this result can be rigorously demonstrated from the properties of Fourier-Bessel functions (Maystre 2002), we shall content ourselves with admitting that the field scattered by the \( j^\text{th} \) rod is generated by sources, i.e. by dipoles, located in this rod. Let us note by contrast that Eq. A.23 cannot be extended to the whole space, since the field generated by the dipolar sources located in the other rods (\( \neq j \)) may present singularities inside these rods.

The validity of Eq. A.24 in the whole space outside the \( j^\text{th} \) rod is a decisive property. It entails that the field represented by the coefficients \( b_{l,m} \) actually is the field scattered by the \( j^\text{th} \) rod in the direction of the other rods, which itself is also a part of the field represented by the coefficients \( a_{l,m}^\text{rods} \ l \neq j \). Hence, if we now consider the balance of the total incident field at the \( l^\text{th} \) rod, i.e. if we add the incident source field to the fields scattered by all other rods in the direction of the \( l^\text{th} \) rod, we should now be in the position of expressing the coefficients \( a_{l,m} \ [ \ [-\infty, +\infty \] \) in terms of the coefficients \( a_{l,m}^\text{source} \ m \in [\ -\infty, +\infty \] \) and \( b_{l,m} \ (m \in [-\infty, +\infty], j \neq l) \). For this purpose, it is first necessary to resolve a mathematical problem: indeed, the incident field at the \( j^\text{th} \) rod is expressed in a local coordinate system associated with this rod, whereas the fields scattered by the other rods are expressed in the local coordinate system associated with these rods.

The representation of all fields in the unique coordinate system associated with the \( l^\text{th} \) rod can be achieved by using Graf’s formula (Abramovitz 1970). This formula expresses in a mathematical form a physically very intuitive result: the field scattered by the \( j^\text{th} \) rod along the direction of the \( l^\text{th} \) rod satisfies in the vicinity of this rod a Helmholtz equation without exhibiting any singularity. This field can therefore be expressed in the form of a Fourier-Bessel series containing only Bessel functions of the first kind. Using the notations presented in Fig. A.1, this formula can be written, in the case where \( r_l(P) \leq r_l^j = O_l O_j \), in the following form:

\[
H^{(1)}_m(k_0 n_{\text{ext}} r_j(P)) \exp(\imath m \theta_j(P)) = \sum_{q=-\infty}^{+\infty} \exp(\imath (m - q) \theta_l^j) H^{(1)}_{q-m}(k_0 n_{\text{ext}} r_l^j) J_q(k_0 n_{\text{ext}} r_l(P)) \exp(\imath q \theta_l(P))
\]  

(Eqs. A.24 and A.25 allow expressing the field scattered by the \( j^\text{th} \) rod in the direction of the \( l^\text{th} \) rod in the coordinate system with origin \( O_l \). Therefore, in the case where \( r_l(P) \leq r_l^j - R \):
\[ E^{d}_{\zeta,i}(P) = \sum_{m=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} b_{j,m} \exp\left( i(m-q)\theta^j_i \right) H^{(1)}_{q-m} \left( k_0 n_{\text{ext}} r^j_i \right) J_q \left( k_0 n_{\text{ext}} r^j_i(P) \right) \exp(iq\theta_i(P)) \] (A.26a)

or, by reversing the indices \( m \) and \( q \):

\[ E^{d}_{\zeta,i}(P) = \sum_{q=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} b_{j,q} \exp\left( i(q-m)\theta^j_i \right) H^{(1)}_{m-q} \left( k_0 n_{\text{ext}} r^j_i \right) J_m \left( k_0 n_{\text{ext}} r^j_i(P) \right) \exp(im\theta_i(P)) \] (A.26b)

The field \( E^{\text{rods}}_{\zeta,j} \) in the ring surrounding the \( l \)th rod, which is obtained by replacing the index \( j \) by the index \( l \) in Eq. A.23, can be identified to the sum of the fields scattered by the \( N - 1 \) other rods \( \sum_{j\neq l} E^{d}_{\zeta,j} \). The sum of these fields can be deduced from equations similar to Eq. A.26b. This identification leads to the following equation:

\[ a^{\text{rods}}_{i,m} = \sum_{j\neq l} \sum_{q=-\infty,\,\infty} b_{j,q} \exp\left( i(q-m)\theta^j_i \right) H^{(1)}_{m-q} \left( k_0 n_{\text{ext}} r^j_i \right) \] (A.27)

Adding the coefficient \( a^{\text{source}}_{i,m} \) of the source field given by Eq. A.22 to the coefficients \( a^{\text{rods}}_{j,m} \), \( a_{i,m} \) can be expressed in terms of the coefficients \( b_{j,q} \) of the fields scattered by the other rods:

\[ a_{i,m} = \left(-1\right)^{m} \exp\left( ik_0 n_{\text{ext}} r^l \sin\left( \Theta^{\text{inc}} - \theta^l \right) - im\Theta^{\text{inc}} \right) \] (A.28)


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