Quantum optics and multiple scattering in dielectrics

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Appendix A

Analytical expression for T-matrix of N-plane crystal

Inversion. The problem that arose in section 2.3.2 and which is solved in this appendix is how to find the inverse of the matrix

\[
M = \begin{pmatrix}
\nu & x & x^2 & x^3 \\
x & \nu & x & x^2 \\
x^2 & x & \nu & x \\
x^3 & x^2 & x & \nu
\end{pmatrix}. \quad (A.1)
\]

The solution will be for general \( N \), but matrices are presented for \( N = 4 \). Define the upper diagonal matrix \( U \) and lower diagonal matrix \( L \) as

\[
U = \begin{pmatrix}
0 & x & 0 & 0 \\
0 & 0 & x & 0 \\
0 & 0 & 0 & x \\
0 & 0 & 0 & 0
\end{pmatrix}; \quad L = \begin{pmatrix}
0 & 0 & 0 & 0 \\
x & 0 & 0 & 0 \\
0 & x & 0 & 0 \\
0 & 0 & x & 0
\end{pmatrix}. \quad (A.2)
\]

Then we have

\[
U^2 = \begin{pmatrix}
0 & 0 & x^2 & 0 \\
0 & 0 & 0 & x^2 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}; \quad U^N = 0. \quad (A.3)
\]

and similarly for powers of the lower diagonal matrix \( L \). From this, it follows that we can write the matrix \( M \) as

\[
M = \nu \mathbb{1} + \sum_{p=1}^{N-1} (U^p + L^p)
= \nu \mathbb{1} + U(\mathbb{1} - U)^{-1} + (\mathbb{1} - L)^{-1} L. \quad (A.4)
\]
Now consider the inverse of the matrix product $(\mathbb{1} - L)M(\mathbb{1} - U)$. Use this and equation (A.4) to arrive at the following expression for the inverse of $M$:

$$M^{-1} = (\mathbb{1} - U)[\nu(\mathbb{1} - L)(\mathbb{1} - U) + (\mathbb{1} - L)U + L(\mathbb{1} - U)]^{-1}(\mathbb{1} - L). \quad (A.5)$$

In this form, finding the inverse is much easier than before, because the matrix has only nonzero elements on the diagonal and first off-diagonals. This becomes clearer by rewriting

$$M^{-1} = (\mathbb{1} - U)[Y + Z]^{-1}(\mathbb{1} - L) = (\mathbb{1} - U)[\mathbb{1} + Y^{-1}Z]^{-1}Y^{-1}(\mathbb{1} - L). \quad (A.6)$$

where $Y \equiv (\nu + \nu x^2 - 2x^2)\mathbb{1} + (1 - \nu)(U + L)$ is a symmetric band diagonal matrix and the matrix $Z$ has matrix elements $Z_{kl} \equiv (2 - \nu)x^p \delta_{kl} \delta_{p1}$ so that only its upper left element is nonzero.

The matrix $M^{-1}$ is known when $Y^{-1}$ and $[\mathbb{1} + Y^{-1}Z]^{-1}$ are known. Now $Y$ has a simple structure and it can be inverted immediately using the transformation matrix $J_{kl} \equiv \sqrt{2/(N + 1)} \sin[kl\pi/(N + 1)]$. It is its own inverse and it diagonalizes $Y$: we have $Y^{-1} = JA^{-1}J$ with $A^{-1} = \delta_{kl}f^{-1}(k)$ where the function $f(k)$ is defined as

$$f(k) \equiv \nu(1 + x^2 - 2x^2 + 2x(1 - \nu)\cos[k\pi/(N + 1)] \quad (k = 1, 2, \ldots, N). \quad (A.7)$$

What remains to be done for the inversion of $M$ is the evaluation of the infinite series

$$(\mathbb{1} + Y^{-1}Z)^{-1} = \mathbb{1} - Y^{-1}Z + (Y^{-1}Z)^2 - (Y^{-1}Z)^3 + \ldots \quad (A.8)$$

Now since we have

$$(Y^{-1}Z)_{kp} = (2 - \nu)x^p \sum_{m=1}^{N} J_{km}f^{-1}(m)J_{mp} \equiv h_N(k, p)\delta_{1p}. \quad (A.9)$$

where in the last equality the function $h_N(k, p)$ was defined, we find that $[(Y^{-1}Z)^n]_{kp} = h_N(k, 1)h_N^{-1}(1, 1)\delta_{1p}$. Summing up all orders, we find that

$$(\mathbb{1} + Y^{-1}Z)^{-1}_{kp} = \left[\delta_{kp} - \left(\frac{h_N(k, 1)}{1 + h_N(1, 1)}\right)\delta_{1p}\right]. \quad (A.10)$$

Inserting this into equation (A.6), we have found the inverse of the matrix $M$. This result is used in equation (2.30) of section 2.3.2.

**Symmetry.** The T-matrix elements should have the symmetry $T_{\alpha, \beta}^{(N)} = T_{N+1-\alpha, N+1-\beta}^{(N)}$, but in the expression (2.30) for the T-matrix that was used in the calculations, this symmetry is not manifest, as was remarked in section 2.5. Here we show how the hidden symmetry can be pulled out.

All terms in Eq. (2.30) should be brought under one denominator. Rewrite the sines and cosines in the expressions in terms of complex exponentials and introduce new variables for the exponentials such that the expression becomes a polynomial in the new variables. In this form it is easier to find that the nominator and denominator have the common
factors \([x - \exp(i Ka)]\) and \([x - \exp(-i Ka)]\) that can be divided out. For the T-matrix we then find
\[
T^{(N)}_{\alpha\beta} = \frac{i k_z \left[ x^2 - 2x \cos(Ka) + 1 \right]^2}{x(x^2 - 1) \sin(Ka)} H^{(N)}_{\alpha\beta}.
\] (A.11)

with \(H^{(N)}_{\alpha\beta}\) for \(\alpha > \beta\) defined as
\[
H^{(N)}_{\alpha\beta} \equiv \frac{x \sin[(\alpha - N)Ka] - \sin[(\alpha - N - 1)Ka]}{x \cos[(N - 1)Ka/2] - \cos((N + 1)Ka/2)} \times \frac{x \sin[(\beta - 1)Ka] - \sin[\beta Ka]}{x \sin[(N - 1)Ka/2] - \sin[(N + 1)Ka/2]}.
\] (A.12)

For \(\alpha < \beta\) the \(\alpha\) and \(\beta\) should be interchanged in this expression. When \(\alpha = \beta\), it can be shown that an \(\alpha\)-independent term \(\Delta H_{\alpha\alpha}\) should be added to the expression for \(H_{\alpha\beta}\):
\[
\Delta H_{\alpha\alpha} = \frac{-x[x^2 - 2x \cos(Ka) + 1]^{-1} \left[ x \cos(Ka) - 1 \right]^2}{x \cos[(N - 1)Ka/2] - \cos((N + 1)Ka/2)} \times \frac{x^2 \sin[(N - 1)Ka] - 2x \sin(NKa) + \sin[(N + 1)Ka]}{x \sin[(N - 1)Ka/2] - \sin[(N + 1)Ka/2]}.
\] (A.13)

From Eqs. (A.12) and (A.13) we can infer that \(H^{(N)}_{\alpha\beta} = H^{(N)}_{N+1-\alpha,N+1-\beta}\), where it is important to notice that \(N + 1 - \alpha < N + 1 - \beta\) when \(\alpha > \beta\). It follows that also the T-matrix has the required symmetry: \(T^{(N)}_{\alpha\beta} = T^{(N)}_{N+1-\alpha,N+1-\beta}\).

**Determinant.** For section 2.4.2 it is useful to compute the determinant of the matrix \(M\) and this can be done best using equation (A.6): \(\det(M) = \det[Y(1 + Y^{-1}Z)]\). This determinant is equal to \([1 + h_N(1,1)]\) times the product of all the \(f(k)\)'s of equation (A.7).

With equation (2.32) and the definition of the Bloch wave vector this gives
\[
\det[M(k|\omega)] = \left[ \frac{-1}{2x(1 - \nu)} \right]^N \sin[(N + 1)Ka] \left[ \frac{(2 - \nu)x}{1 - \nu} \right] \sin[NKa] \times \prod_{m=1}^N \left[ \cos(Ka) - \cos \left( \frac{m\pi}{N+1} \right) \right] \sin[(N + 1)Ka].
\] (A.14)

Notice that the zeroes of the determinant are not caused by the products of \(\cos(Ka) - \cos \left( \frac{m\pi}{N+1} \right)\) going to zero, because of the \(\sin[(N + 1)Ka]\) in the denominator. The determinant is zero when the remaining factor in the nominator is zero, which is equivalent to \([1 + h_N(1,1)] = 0\).