1D band structure of single periodic scatterer in Schrödinger equation

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Abstract

We give an analytic solution for periodic unit cell containing a single point scatterer in 1D. We also compare the boundary-collocation approach and the lattice-sum approach, in order to look for linearization tricks in the lattice-sum coefficients—we find none.

We consider the following Schrödinger eigenvalue problem,

$$
\begin{aligned}
(\partial_{xx} + \omega^2 - \epsilon\delta(x))u(x) &= 0 \qquad x \in [-\pi, \pi) \qquad \text{(PDE)} & (1)\\
u(\pi) &= \alpha u(-\pi) \qquad \text{(value quasi-periodicity)} & (2)\\
u'(\pi) &= \alpha u'(-\pi) \qquad \text{(derivative quasi-periodicity)} & (3)
\end{aligned}
$$

where $\alpha \in \mathbb{C}$ is the Bloch phase factor, $|\alpha| = 1$. The potential is a delta-distribution of strength ϵ, repulsive for $\epsilon > 0$. The overall wavenumber is $\omega > 0$. By integrating through 0 we see that the PDE (1) is equivalent to the piecewise Helmholtz problem

$$
\begin{aligned}
(\partial_{xx} + \omega^2)u(x) &= 0 \qquad x \in [-\pi, 0) \cup (0, \pi) & (4)\\
[u]_0 := u(0^+) - u(0^-) &= 0 \qquad\qquad \text{(value jump relation)} & (5)\\
[u']_0 := u'(0^+) - u'(0^-) &= \epsilon u(0) \qquad \text{(derivative jump relation)} & (6)
\end{aligned}
$$

This model is chosen since it is simpler than any piecewise-constant dielectric problem for Helmholtz (and is the limit of a vanishingly small dielectric region of large index). By tiling the real line we see that the eigenvalue problem is equivalent to the solution of non-trivial Bloch waves of the form $u(x) = U(x)e^{ikx}$ where U is 2π-periodic and $\alpha = e^{2\pi ik}$, where $k \in [-1/2, 1/2]$ is the (real) Bloch wavevector.

0.1 Analytic solution

Any solution to the Helmholtz equation in an interval is a linear combination of left and right traveling waves $e^{\pm i\omega x}$. One may check that the following basis $\{u^+, u^-\}$ satisfies (4), (2) and (3),

$$
u^\pm(x) = \begin{cases} \overline{\alpha}e^{\pm i\omega(x+2\pi)} & x < 0 \\ e^{\pm i\omega x} & x > 0 \end{cases} \tag{7}
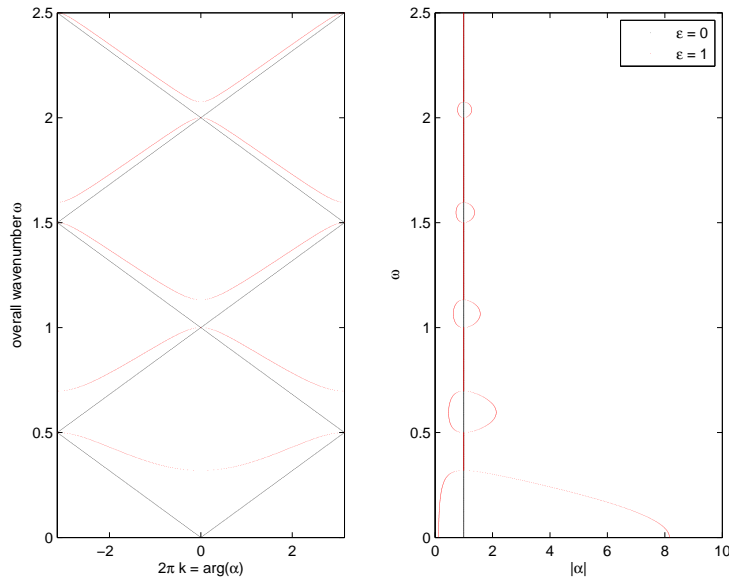$$

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Figure 1: 1D band structure for $\epsilon = 0$ (black lines) and $\epsilon = 1$ (red lines)

We write the general solution as $u(x) = Au^+(x) + Bu^-(x)$ in which case the jump conditions can be written as the two rows of the homogeneous equation

$$M \begin{bmatrix} A \\ B \end{bmatrix} := \begin{bmatrix} 1 - \overline{\alpha}e^{2\pi i \omega} & 1 - \overline{\alpha}e^{-2\pi i \omega} \\ 1 - \overline{\alpha}e^{2\pi i \omega} + i\frac{\epsilon}{\omega} & -1 + \overline{\alpha}e^{-2\pi i \omega} + i\frac{\epsilon}{\omega} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (8)$$

Since the matrix M is linear in $\overline{\alpha}$, this is a 2-by-2 matrix generalized eigenvalue problem. Equivalently, nontrivial solutions exist when $\det M = 0$, which gives the following quadratic equation in $\overline{\alpha}$,

$$\overline{\alpha}^2 - 2b\overline{\alpha} + 1 = 0 \qquad \text{where} \quad b(\omega, \epsilon) := \cos 2\pi\omega + \frac{\epsilon}{2\omega} \sin 2\pi\omega \qquad (9)$$

We immediately see that the product of the two roots is 1. Solutions are

$$\overline{\alpha} = b \pm \sqrt{b^2 - 1} \qquad (10)$$

which lie on the unit circle (and are conjugates) iff $|b| \leq 1$. The phase (angle) of α is $2\pi k$, obeys $\cos 2\pi k = b$, and is shown in Fig. 1a. With $\epsilon = 0$ (empty unit cell) we get $k = \pm\omega + n$, for $n \in \mathbb{Z}$. Note that increasing ϵ tends to push the band ω values higher. When $|b| > 1$ there is a bandgap, and the roots move away from 1 along the real axis, as shown in Fig. 1b. This would correspond to growing/decaying evanescent rather than Bloch waves. The ω values at the upper band edges $|b| = 1$ are solutions to a transcendental equation.

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0.2 Boundary matching method

The Greens function for the free-space 1D Helmholtz equation $(\partial_{xx} + \omega^2)u(x) = f$ is

$$G(x) = -\frac{1}{2\omega} \sin \omega |x| \tag{11}$$

For $\omega \neq 0$ this satisfies $[G]_0 = 0$ and $[G']_0 = -1$. A trial solution satisfying (4) and (5) is

$$u(x) = ae^{i\omega x} + be^{-i\omega x} + cG(x) \tag{12}$$

The value and derivative QP condition (2), (3), and the derivative jump relation (6) at the scatterer, give the 3 rows of the homogeneous matrix equation where $\beta := e^{i\omega \pi}$,

$$Q \begin{bmatrix} a \\ b \\ c \end{bmatrix} := \begin{bmatrix} \beta\overline{\alpha} - \overline{\beta} & \overline{\beta}\overline{\alpha} - \beta & \frac{\overline{\alpha}-1}{4i\omega}(\overline{\beta} - \beta) \\ \beta\overline{\alpha} - \overline{\beta} & -\overline{\beta}\overline{\alpha} + \beta & -\frac{\overline{\alpha}+1}{4i\omega}(\overline{\beta} + \beta) \\ \epsilon & \epsilon & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{13}$$

Bloch eigenfunctions correspond to nontrivial solutions of the above. By subtracting row 1 from row 2, then subtracting column 1 from column 2, we get, performing some tedious algebra,

$$\det Q = \begin{bmatrix} \beta\overline{\alpha} - \overline{\beta} & (1 + \overline{\alpha})(\overline{\beta} - \beta) & \frac{\overline{\alpha}-1}{4i\omega}(\overline{\beta} - \beta) \\ 0 & -2(\overline{\beta}\overline{\alpha} - \beta) & -2(\overline{\beta}\overline{\alpha} + \beta) \\ \epsilon & 0 & 1 \end{bmatrix} = -2(\overline{\alpha}^2 - 2b\overline{\alpha} + 1) \tag{14}$$

which being a nonzero multiple of the LHS of (9) shows that $\det Q = 0 \Leftrightarrow \det M = 0$; the two formulations are equivalent. Note that since the last row of Q does not involve $\overline{\alpha}$, the determinant is quadratic rather than cubic in $\overline{\alpha}$. Since Q is linear in $\overline{\alpha}$, (13) could instead be written as a 3-by-3 generalized eigenvalue problem with $\overline{\alpha}$ the eigenvalue.

0.3 Lattice sum method

We quasi-periodize the Greens function (11) to get a solution to (4), (2) and (3),

$$G_{\text{QP}}(x) = \sum_{n \in \mathbb{Z}} \alpha^n G(x - 2\pi n) = G(x) + s^+ e^{i\omega x} + s^- e^{-i\omega x} \tag{15}$$

where we have written the contribution from $n \neq 0$ using the complete basis for regular Helmholtz solutions in the unit cell. This can be solved for analytically, but convergence of the sums requires regularization, as we see below. This defines the lattice sums (plane wave coefficients) s^+, s^- which we get by evaluating, taking care with the absolute value signs,

$$\sum_{n \in \mathbb{Z}} \alpha^n G(x - 2\pi n) = \frac{i}{4\omega} \left[\sum_{n>0} e^{2\pi i n k} \left(e^{2\pi i n \omega - ikx} - e^{-2\pi i n \omega + ikx} \right) + \sum_{n<0} e^{2\pi i n k} \left(e^{-2\pi i n \omega + ikx} - e^{2\pi i n \omega - ikx} \right) \right]$$

$$\tag{16}$$

The coefficient of $e^{i\omega x}$ is, summing the geometric series in the limit $\omega \to 0^-$ for $n > 0$ and $\omega \to 0^+$ for $n < 0$, with k real (so $|\alpha| = 1$),

$$
\begin{aligned}
s^+ &= \frac{i}{4\omega}\left[-\sum_{n>0} e^{2\pi in(k-\omega)} + \sum_{n<0} e^{2\pi in(k-\omega)}\right] \\
&= \frac{i}{4\omega}\left[-\frac{\alpha e^{-2\pi i\omega}}{1 - \alpha e^{-2\pi i\omega}} + \frac{\overline{\alpha} e^{2\pi i\omega}}{1 - \overline{\alpha} e^{2\pi i\omega}}\right] \\
&= -\frac{1}{2\omega}\mathrm{Im}\frac{1}{1 - \overline{\alpha} e^{2\pi i\omega}}
\end{aligned}
\tag{17}
$$

Similarly we get

$$
s^- = \frac{1}{2\omega}\mathrm{Im}\frac{1}{1 - \overline{\alpha} e^{-2\pi i\omega}}
\tag{18}
$$

We see that s^+ (s^-) diverges to infinity only on the negative (positive) sloping parts of the $\epsilon = 0$ band structure $k = -\omega + n$ $(k = \omega + n)$, $n \in \mathbb{Z}$. This divergence is not physically related to the band structure at any other $\epsilon \neq 0$, yet poses a difficulty inherent to the method.

Since we have periodized the Greens function, only the condition at the scatterer need be solved. Since G_{QP} already satisfies (5), the only remaining condition is the derivative jump (6), giving via (17) and (18),

$$
-1 = \epsilon(s^+ + s^-) = \frac{\epsilon}{2\omega}\,\mathrm{Im}\frac{-2i\overline{\alpha}\sin 2\pi\omega}{1 - 2\overline{\alpha}\cos 2\pi\omega + \overline{\alpha}^2}
\tag{19}
$$

Remarkably, the expression whose imaginary part is to be taken is pure imaginary, as can be shown by multiplying top and bottom by the conjugate of the bottom and simplifying to

$$
-2i\sin 2\pi\omega\frac{\overline{\alpha} + \alpha - 2\cos 2\pi\omega}{2 + 4\cos^2 2\pi\omega - 4(\overline{\alpha} + \alpha)\cos 2\pi\omega + \overline{\alpha}^2 + \alpha^2}
\tag{20}
$$

There is a simple geometric understanding of this: for any ω and k, we have Re $s^- = -$ Re $s^+ = 1/2$, from the fact that $\overline{\alpha}e^{\pm 2i\pi\omega}$ lie on the unit circle, and any circle touching 0 inverts to a straight line. Therefore Im can be replaced by $-i$ turning (19) into

$$
-1 = \frac{\epsilon}{2\omega}\frac{-2\overline{\alpha}\sin 2\pi\omega}{1 - 2\overline{\alpha}\cos 2\pi\omega + \overline{\alpha}^2}
\tag{21}
$$

which is identical to the original analytic solution (9).

0.4   Conclusion

The lattice sums are not linear in the Bloch factor α, since summing the geometric (Neumann) series results in inversion. In contrast, boundary matching (the method used by Hafner *et al.* at ETH) can be phrased as a linear generalized eigenvalue problem in α. In this simple setting we have shown that the methods are equivalent and reproduce the analytic solution.

A Code for figure

```
Ks = 0:.002:2.5;                                   % overall omega wavenumbers
ab = NaN*ones(2,numel(Ks));                        % alphas of band struct
epss = 0:1:1;                                       % eps values
figure;
for i=1:numel(epss)
  eps = epss(i);
  for j=1:numel(Ks)
    K = Ks(j);
    tb = cos(2*pi*K) + eps*sin(2*pi*K)./K/2;  % -2b in quadratric eqn for alpha
    sd = sqrt(tb*tb - 1);                          % discriminant (a=c=1)
    ab(1,j) = tb + sd; ab(2,j) = tb - sd;      % pair of roots
  end
  subplot(1,2,1); plot(angle(ab)./(abs(abs(ab)-1)<1e-10), Ks, '.', ...
                       'markersize', 1, 'color', [i-1 0 0]);
  hold on; xlabel('2\pi k = arg(\alpha)'); ylabel('overall wavenumber \omega');
  axis([-pi pi 0 max(Ks)]);
  subplot(1,2,2); plot(abs(ab), Ks, '.', ...
                       'markersize', 1, 'color', [i-1 0 0]);
  hold on; xlabel('|\alpha|'); ylabel('\omega');
end
[l h] = legend('\epsilon = 0', '\epsilon = 1'); set(h(6), 'color', [1 0 0]);
```