Appendix A
The Kronig–Penney Model

The Kronig–Penney model [1] played a significant and unique role in our current understanding of the electronic states in one-dimensional crystals [2–7]. Naturally, the model has also been playing an important role in various problems in solid state physics. An interesting point of the Kronig–Penney model is that not only the band structure of a Kronig–Penney crystal can be analytically obtained as well known in the solid state physics community, but also the function formalisms of all solutions, both in the permitted and forbidden energy ranges, can be analytically obtained and explicitly expressed. This point provides a significant convenience for using this model as a concrete example to illustrate the mathematical theory in Part II. This appendix is organized as follows: In Sect. A.1, we briefly describe the model. In Sect. A.2, we use the theory in Chap. 2 to obtain the band structure of the model. In Sect. A.3, the function formalisms of all solutions of a Kronig–Penney crystal in various energy ranges are obtained to illustrate the theory in Chap. 2. In Sect. A.4, a semi-infinite Kronig–Penney crystal is treated, the existence and properties of surface states are investigated based on the theory in Chap. 3 and compared with the classical results obtained by Tamm [5] and described by Seitz in his classic book [2]. Finally, in Sect. A.5 are the results for the Kronig–Penney crystal of finite length \( L = Na \) and comparisons with the theory in Chap. 4.

A.1 The Model

The Schrödinger equation for an electron moving in a one-dimensional potential \( U(x) \) can be written as [5]

\[
y''(x) + \chi^2[\lambda - U(x)]y(x) = 0, \quad \chi^2 = \frac{8\pi^2m}{h^2}, \quad (A.1)
\]

where \( \lambda \) is the energy. In the Kronig–Penney model a one-dimensional crystal with a rectangular potential \( U(x) \) of the period \( a \) is investigated, where two potential
regions with length $d_1$ and $d_2$ exist in each unit cell. In the $\ell$th unit cell of the crystal, $a(\ell - 1) \leq x \leq a\ell$ – here $\ell$ is an integer, the rectangular potential $U(x)$ can be written as

$$U(x) = \begin{cases} 0, & 0 \leq x - a(\ell - 1) \leq d_1, \\ U_2, & d_1 \leq x - a(\ell - 1) \leq d_1 + d_2, \end{cases} \quad \text{(A.2)}$$

where $d_1 + d_2 = a$ and $U_2$ is a positive real constant.

Further in the Kronig–Penney limit that

$$\lim d_2 = 0, \quad \lim d_1 = a, \quad \lim U_2 = \infty,$$

and keeping

$$\lim(U_2d_2) = p = \text{Const}, \quad \text{(A.3)}$$

the Schrödinger equation (A.1) becomes

$$-y''(x) + \left[ \sum_{n=\infty}^{\infty} \frac{2p}{a} \delta(x - na) - \frac{\xi^2}{a^2} \right] y(x) = 0, \quad -\infty < x < \infty \quad \text{(A.4)}$$

where

$$\xi = a\chi \sqrt{\lambda}. \quad \text{(A.5)}$$

In this Appendix, it is more convenient to discuss $\xi$ instead of $\lambda$ in many cases, similar in [5]. We will treat $\xi$ rather than $\lambda$ in most equations.

### A.2 Normalized Solutions and the Discriminant

#### A.2.1 Normalized Solutions

We are interested in the properties of solutions of Eq. (A.4) in the interval $[-\frac{a}{2}, \frac{a}{2}]$. Two normalized solutions $\eta_1(x, \xi)$ and $\eta_2(x, \xi)$ of Eq. (A.4) are defined by the conditions that

$$\eta_1\left(-\frac{a}{2}, \xi\right) = 1, \eta_1'\left(-\frac{a}{2}, \xi\right) = 0; \quad \eta_2\left(-\frac{a}{2}, \xi\right) = 0, \eta_2'\left(-\frac{a}{2}, \xi\right) = 1. \quad \text{(A.6)}$$

By integrating Eq. (A.4) from $-\varepsilon$ to $\varepsilon$ where $\varepsilon$ is an infinitely small positive number, for any solution $y$ of Eq. (A.4) we have

$$y'(\varepsilon) - y'(-\varepsilon) = 2 \frac{p}{a} y(0). \quad \text{(A.7)}$$
Two normalized solutions of Eq. (A.4) can be obtained as
\[
\eta_1(x, \xi) = \begin{cases} 
\cos \frac{\xi}{2} \cos \frac{\xi}{a} x - \sin \frac{\xi}{2} \sin \frac{\xi}{a} x, & -\frac{a}{2} \leq x < 0, \\
\cos \frac{\xi}{2} \cos \frac{\xi}{a} x + \left(2 \frac{p}{\xi} \cos \frac{\xi}{2} - \sin \frac{\xi}{2} \right) \sin \frac{\xi}{a} x, & 0 < x \leq \frac{a}{2},
\end{cases}
\]
(A.8)

and
\[
\eta_2(x, \xi) = \begin{cases} 
\left(\frac{\xi}{a}\right)^{-1} \left(\sin \frac{\xi}{2} \cos \frac{\xi}{a} x + \cos \frac{\xi}{2} \sin \frac{\xi}{a} x\right), & -\frac{a}{2} \leq x < 0, \\
\left(\frac{\xi}{a}\right)^{-1} \left[\sin \frac{\xi}{2} \cos \frac{\xi}{a} x + \left(\cos \frac{\xi}{2} + 2 \frac{p}{\xi} \sin \frac{\xi}{2}\right) \sin \frac{\xi}{a} x\right], & 0 < x \leq \frac{a}{2},
\end{cases}
\]
(A.9)

where Eqs. (A.6) and (A.7) were used.

From Eqs. (A.8) and (A.9) we obtain that
\[
\eta_1 \left(\frac{a}{2}, \xi\right) = \cos \xi + \frac{p}{\xi} \sin \xi, \quad \eta_1' \left(\frac{a}{2}, \xi\right) = -\frac{\xi}{a} \left(\sin \xi - 2 \frac{p}{\xi} \cos^2 \frac{\xi}{2}\right),
\]
\[
\eta_2 \left(\frac{a}{2}, \xi\right) = \left(\frac{\xi}{a}\right)^{-1} \left(\sin \xi + 2 \frac{p}{\xi} \sin^2 \frac{\xi}{2}\right), \quad \eta_2' \left(\frac{a}{2}, \xi\right) = \cos \xi + \frac{p}{\xi} \sin \xi.
\]
(A.10)

\subsection{The Discriminant $D(\xi)$}

From Eq. (A.10) we obtain the discriminant $D(\xi)$ of Eq. (A.4) as
\[
D(\xi) = \eta_1 \left(\frac{a}{2}, \xi\right) + \eta_2' \left(\frac{a}{2}, \xi\right) = 2 \cos \xi + 2 \frac{p}{\xi} \sin \xi.
\]
(A.11)

In each energy range where $-2 \leq D(\xi) \leq 2$, we obtain Bloch wave functions $\phi_n(\pm k, x)$ as eigensolutions of (A.4):
\[
\phi_n(\pm k, x + a) = e^{\pm ika} \phi_n(\pm k, x),
\]
(A.12)

where $-\pi/a < k \leq \pi/a$. The Bloch wave vector $k$ and $\xi$ are related by (2.74) as:
\[
\cos ka = \cos \xi + \frac{p}{\xi} \sin \xi.
\]
(A.13)

This is the well-known band structure equation for the Kronig–Penney model [1–3]. Although this band structure of the Kronig–Penney model has been well known for many years, the approach used here is easier to be extended to treat more general and complicated cases, such as that there are more than two potential regions in one period: $a = d_1 + d_2 + d_3 \ldots$, each region has a different width and a different potential height, and so forth.
The energy ranges where \( D(\xi) < -2 \) are band gaps at \( k = \pi/a \). Two linearly independent solutions of the Eq. (A.4) can be written as \( (\beta > 0) \):

\[
y(\xi, \pm \beta, x + a) = -e^{\pm \beta a} y(\xi, \pm \beta, x), \quad -\infty < x < +\infty, \quad (A.14)
\]

where \( \beta \) and \( \xi \) are related by (2.82):

\[
cosh \beta a = -\cos \xi - \frac{p}{\xi} \sin \xi. \quad (A.15)
\]

The energy ranges where \( D(\xi) > 2 \) are band gaps at \( k = 0 \). Two linearly independent solutions of the Eq. (A.4) can be written as \( (\beta > 0) \):

\[
y(\xi, \pm \beta, x + a) = e^{\pm \beta a} y(\xi, \pm \beta, x), \quad -\infty < x < +\infty, \quad (A.16)
\]

where \( \beta \) and \( \xi \) are related by (2.78):

\[
cosh \beta a = \cos \xi + \frac{p}{\xi} \sin \xi. \quad (A.17)
\]

Unlike in (A.12) where the Bloch wave vector \( k \) is a monotonic function of \( \xi \) in a specific permitted band, thus, a pair of \( \pm k \) can only correspond to one unique \( \xi \). \( \beta \) is not a monotonic function of \( \xi \) in a specific band gap, so one pair of \( \pm \beta \) may correspond to two different \( \xi \). Therefore, in (A.14) and (A.16) \( \xi \) is needed to specify a solution in a band gap.

### A.2.3 The Band Edge Eigenvalues

The upper edge of the \( n \)th permitted band—that is the lower edge of the \( n \)th band gap, and it can be denoted as \( \omega_n \)—is at

\[
\xi = \omega_n = (n + 1)\pi. \quad n = 0, 1, 2, 3, \ldots \quad (A.18)
\]

The lower edge of the \( n \)th permitted band—that is the upper edge of the \( n - 1 \)th band gap if \( n > 0 \)—is at

\[
\begin{align*}
\frac{\xi}{2} \tan \frac{\xi}{2} &= p/2, & n &= 0, 2, 4, \ldots, \\
\frac{\xi}{2} \cot \frac{\xi}{2} &= -p/2, & n &= 1, 3, 5, \ldots.
\end{align*} \quad (A.19)
\]

Those are well-known results [1, 3, 7]. The upper edge of the \( n \)th band gap can be denoted as \( \Omega_n, n = 0, 1, 2, 3, \ldots \).

The band structure of a Kronig–Penney crystal depends on \( p \) in (A.4). The band edges determined by (A.18) and (A.19) are shown in Fig. A.1, as functions of \( p \).
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In the following, in most cases $p = \frac{3\pi}{2}$ is assumed as in [1, 5]. Nevertheless, we will see that in some cases the physical results in the Kronig–Penney model might significantly even qualitatively depend on the value of $p$.

A.3 Solutions of the Differential Equation

In the following, we obtain the solutions of the differential equation (A.4). We consider three different cases:

1. $\xi$ is inside a permitted band;
2. $\xi$ is at a band edge: $\xi = \omega_n$ or $\xi = \Omega_n$;
3. $\xi$ is inside a band gap: $\omega_n < \xi < \Omega_n$.

We only need to obtain the solutions in one period $[-\frac{a}{2}, \frac{a}{2}]$. This is the reason we choose the two normalized solutions $\eta_1(x, \xi)$ and $\eta_2(x, \xi)$ of Eq. (A.4) according to (A.8). In general, a solution of Eq. (A.4) in the interval $[-\frac{a}{2}, \frac{a}{2}]$ can be written as a linear combination of two normalized solutions $\eta_1(x, \xi)$ and $\eta_2(x, \xi)$:

$$y(x, \xi) = c_1 \eta_1(x, \xi) + c_2 \eta_2(x, \xi), \quad -\frac{a}{2} \leq x \leq \frac{a}{2}. \quad (A.20)$$

Since $\eta_1(x, \xi)$ and $\eta_2(x, \xi)$ were given in (A.8)–(A.9), the solution can be determined—with a normalization constant factor difference—if $\frac{c_2}{c_1}$ in each different case is determined.
The solutions in the whole real axis \((-\infty < x < +\infty)\) can be obtained by using Eqs. (A.12), (A.14), or (A.16).

The understandings of the zeros of solutions of periodic differential equations play a fundamental role in the theory in Chap. 4. We will pay particular attention to the zeros of solutions of Eq. (A.4) for \(\xi\) in different cases.

### A.3.1 \(\xi\) Is Inside a Permitted Band

When \(\xi\) is inside a permitted band, the solutions of (A.4) are Bloch wave functions \(\phi_n(\pm k, x)\) \((0 < k < \pi/a)\) as in (A.12). By using \(x = -\frac{a}{2}\) in (A.12) and writing \(\phi_n(\pm k, x)\) in the form (A.20) with (A.10), we obtain that

\[
\frac{c_2}{c_1} = \pm \sqrt{\frac{D - 2}{D + 2} \frac{\xi}{a} \cos \frac{\xi}{2}},
\]

where \(D\) is the discriminant (A.11). Thus inside a permitted band of Eq. (A.4), the Bloch wave functions \(\phi_n(\pm k, x)\) have the form

\[
\phi_n(\pm k, x) = C \left[ \sqrt{D + 2} \sin \frac{\xi}{2} \eta_1(x, \xi) \pm \sqrt{D - 2} \frac{\xi}{a} \cos \frac{\xi}{2} \eta_2(x, \xi) \right],
\]

\[-\frac{a}{2} \leq x \leq \frac{a}{2},\]

where \(C\) is a normalization constant.

Note that as a solution of (A.4) with \(\xi\) inside a permitted band, \(\phi_n(\pm k, x)\) in Eq. (A.22) does not have zeros. Neither \(\sin \frac{\xi}{2}\) nor \(\cos \frac{\xi}{2}\) can be zero; \(\sqrt{D + 2}\) is a non-zero real number, but \(\sqrt{D - 2}\) is a non-zero imaginary number; and, \(\eta_1(x, \xi)\) and \(\eta_2(x, \xi)\) are real functions not being zero simultaneously, due to the Sturm Separation Theorem.

### A.3.2 \(\xi\) Is at a Bandedge: \(\xi = \omega_n\) Or \(\xi = \Omega_n\)

The wave function for \(\xi\) being at a band-edge can be easier obtained by noticing that \(\phi_n(\pm k, x)\) is either a real symmetric function or a real antisymmetrical function due to the inversion symmetry of Eq. (A.4).

Since the potential is zero in the region except the delta-function barrier at \(x = 0\), the real symmetrical solution for a specific \(\xi\) of the Eq. (A.4) is
Fig. A.2  $c$ in (A.23) as the function of $\xi$. $p = 3\pi/2$ is assumed

$$f_s(\xi, x) = \begin{cases} 
\cos \left[ \frac{\xi}{a} (-x + c) \right], & -a/2 \leq x \leq 0, \\
\cos \left[ \frac{\xi}{a} (x + c) \right], & 0 \leq x \leq a/2.
\end{cases} \quad (A.23)$$

where $c$ is a constant depending on $\xi$ due to the existence of the delta-function barrier indicated in (A.7) and determined by

$$\tan \frac{\xi}{a} c = -\frac{p}{\xi}. \quad (A.24)$$

In Fig. A.2 is shown $c$ in (A.23) as the function of $\xi$, determined by (A.24) for a specific $p = 3\pi/2$.

The real antisymmetrical solution of Eq. (A.4) is

$$f_a(\xi, x) = \sin \frac{\xi}{a} x, \quad -a/2 \leq x \leq a/2. \quad (A.25)$$

Since a band-edge wave function must have $\phi_n(\pi/a, a/2) = -\phi_n(\pi/a, -a/2)$ or $\phi_n(0, a/2) = \phi_n(0, -a/2)$ by Eq. (A.12), it is easy to see that the band-edge wave function at the lower edge $\xi = \omega_n$ of each band gap is an antisymmetrical function:

$$\phi_n(k_g, x) = C \sin \left[ \frac{(n + 1)\pi}{a} x \right], \quad -a/2 \leq x \leq a/2. \quad (A.26)$$

where Eq. (A.18) is used.
The band-edge wave function at the upper edge $\xi = \Omega_n$ of each band gap must be a symmetrical function:

$$\phi_{n+1}(k_g, x) = \begin{cases} C \cos \left[ \frac{\xi}{a} (-x + c) \right], & -a/2 \leq x \leq 0, \\ C \cos \left[ \frac{\xi}{a} (x + c) \right], & 0 \leq x \leq a/2, \end{cases} \quad (A.27)$$

where $n = 0, 1, 2, 3, \ldots$ and $k_g = \pi/a$ or $k_g = 0$ in Eqs. (A.26) and (A.27). Similarly, the band-edge wave function $\phi_0(0, x)$ at the lowest band edge $\varepsilon_0(0)$ must be a symmetrical function since $\phi_0(0, a/2) = \phi_0(0, -a/2)$:

$$\phi_0(0, x) = \begin{cases} C \cos \left[ \frac{\xi}{a} (-x + c) \right], & -a/2 \leq x \leq 0, \\ C \cos \left[ \frac{\xi}{a} (x + c) \right], & 0 \leq x \leq a/2. \end{cases} \quad (A.28)$$

In Eqs. (A.27) and (A.28) $\xi$ is given by Eq. (A.19). $C$ is a normalization constant in Eqs. (A.26), (A.27) and (A.28).

In Fig. A.3 are shown the two band-edge wave functions $\phi_0(\pi/a, x)$ and $\phi_1(\pi/a, x)$ of the lowest band gap at $k = \pi/a$. In Figs. A.3 and A.4, we assume that $C=1$ for simplicity since the normalization constants do not affect the points with which we are concerned here. It can be seen that both the Bloch wave functions $\phi_0(\pi/a, x)$ and $\phi_1(\pi/a, x)$ have one zero in the interval $(-\frac{a}{2}, \frac{a}{2})$, as in Theorem 2.7. (iii).

![Fig. A.3](image-url)
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Fig. A.4 The lowest band-edge wave function \( \phi_0(0, x) \) and two band-edge wave functions \( \phi_1(0, x) \) and \( \phi_2(0, x) \) of the lowest band gap at \( k = 0 \). Note the discontinuity of the derivatives of \( \phi_0(0, x) \) and \( \phi_2(0, x) \) at \( x = 0 \) due to (A.7). Note that \( \phi_0(0, x) \) has no zero, \( \phi_1(0, x) \) has two zeros \( x = 0 \) and \( x = \frac{a}{2} \) (solid circles) in the interval \((-\frac{a}{2}, \frac{a}{2})\); \( \phi_2(0, x) \) has two symmetrical zeros (open circles) in the interval \((-\frac{a}{2}, \frac{a}{2})\).

In Fig. A.4 are shown the lowest band-edge wave function \( \phi_0(0, x) \) and two band-edge wave functions \( \phi_1(0, x) \) and \( \phi_2(0, x) \) of the lowest band gap at \( k = 0 \). It can be seen that \( \phi_0(0, x) \) has no zero in \((-\frac{a}{2}, \frac{a}{2})\), leading to the conclusion that \( \phi_0(0, x) \) has no zero in \((-\infty, +\infty)\) as in Theorem 2.7 (i). Both Bloch wave functions \( \phi_1(0, x) \) and \( \phi_2(0, x) \) have two zeros in the interval \((-\frac{a}{2}, \frac{a}{2})\), as in Theorem 2.7. (ii).

From (A.26) we can see that the wave function \( \phi_n(k_g, x) \) at the lower edge of the \( n \)th band gap has \( n + 1 \) zeros in \((-a/2, a/2)\); Eqs. (A.27) and (A.19) lead to that the wave function \( \phi_{n+1}(k_g, x) \) at the upper edge of the \( n \)th band gap has \( n + 1 \) zeros in \((-a/2, a/2)\), in consistence with Theorem 2.7. (ii) and (iii). The lower band-edge wave function of each gap always has a zero at the potential maximum \( x = 0 \).

A.3.3 \( \xi \) Is Inside A Band Gap

In the following, we consider the solutions of Eq. (A.4) when \( \xi \) is inside a band gap. We need to consider two cases: \( \xi \) is inside a band gap at \( k = \pi/a \) or \( \xi \) is inside a band gap at \( k = 0 \).

A.3.3.1 \( \xi \) Is Inside A Band Gap at \( k = \pi/a \)

The \( \xi \) ranges where \( D(\xi) < -2 \) are band gaps at \( k = \pi/a \). Two linearly independent solutions of the Eq. (A.4) can be written as in the form of (A.14) \((\beta > 0)\); \( y(\xi, \pm\beta, x + a) = -e^{\pm\beta a} y(\xi, \pm\beta, x) \), where \( \beta \) and \( \xi \) are related by (A.15).
By using $x = -a^2$ in (A.14) and writing $y(\xi, \pm \beta, x)$ in the form (A.20) with Eq. (A.10), we obtain that,

$$\frac{c_2}{c_1} = \pm \frac{\xi \cos \frac{\xi}{2}}{\sin \frac{\xi}{2}} \sqrt{\frac{D - 2}{D + 2}},$$

where $D = 2 \cos \xi + 2 \frac{\beta}{\xi} \sin \xi$ is the discriminant of (A.4). Since $D < -2$ for a $\xi$ inside a band gap at $k = \pi/a$, we have

$$y(\xi, \pm \beta, x) = C \left[ \sin \frac{\xi}{2} \sqrt{-D - 2} \eta_1(x, \xi) \pm \frac{\xi}{a} \cos \frac{\xi}{2} \sqrt{2 - D} \eta_2(x, \xi) \right], \quad (A.29)$$

here $C$ is a normalization constant. In this subsection, we choose the normalization constant $C$ of $y(\xi, \pm \beta, x)$ in Eq. (A.29) by requiring $y(\xi, \pm \beta, 0) = 1$. From Eq. (A.29) we obtain that

$$y(\xi, \pm \beta, x) = \begin{cases} \frac{2}{\sin \xi (\sqrt{-D - 2 + \sqrt{2 - D}})} \left[ \sin \frac{\xi}{2} \sqrt{-D - 2} \cos \left( \frac{\xi}{2} + \frac{\xi}{a} x \right) \right. \\
\pm \cos \frac{\xi}{2} \sqrt{2 - D} \sin \left( \frac{\xi}{2} + \frac{\xi}{a} x \right), & -\frac{a}{2} \leq x \leq 0, \\
\frac{2}{\sin \xi (\sqrt{-D - 2 + \sqrt{2 - D}})} \left[ \sin \frac{\xi}{2} \sqrt{-D - 2} \cos \left( \frac{\xi}{2} - \frac{\xi}{a} x \right) \right. \\
\pm \cos \frac{\xi}{2} \sqrt{2 - D} \sin \left( \frac{\xi}{2} - \frac{\xi}{a} x \right), & 0 \leq x \leq \frac{a}{2}. \end{cases}, \quad (A.30)$$

The first part of Eq. (A.30) is directly from Eqs. (A.29) and (A.10), the second part comes from that due to the inversion symmetry of Eq. (A.4), $y(\xi, +\beta, x)$ in the $+x$ direction behaves exactly same as $y(\xi, -\beta, x)$ in the $-x$ direction: $y(\xi, \pm \beta, x) = y(\xi, \mp \beta, -x)$.

**Zeros of Solutions:**

The zeros $x = x_0$ of a solution $y(\xi, \pm \beta, x)$ in (A.30) of Eq. (A.4) for $\xi$ in a band gap at $k = \pi/a$ is determined by

$$y(\xi, \pm \beta, x_0) = 0.$$

Thus the zeros $x = x_0$ of $y(\xi, \pm \beta, x)$ are the solutions of one of the two following equations:

$$\cot \left( \frac{\xi}{2} + \frac{\xi}{a} x_0 \right) = \pm \sqrt{\frac{-\sin \frac{\xi}{2} + \frac{\xi}{a} (1 + \cos \frac{\xi}{2})}{\sin \frac{\xi}{2} + \frac{\xi}{a} (1 - \cos \frac{\xi}{2})}}, \quad -\frac{a}{2} \leq x_0 \leq 0$$

$$\cot \left( \frac{\xi}{2} - \frac{\xi}{a} x_0 \right) = \mp \sqrt{\frac{-\sin \frac{\xi}{2} + \frac{\xi}{a} (1 + \cos \frac{\xi}{2})}{\sin \frac{\xi}{2} + \frac{\xi}{a} (1 - \cos \frac{\xi}{2})}}, \quad 0 \leq x_0 \leq \frac{a}{2}$$

(A.31)
A.3.3.2  \( \xi \) Is Inside A Band Gap at \( k = 0 \)

The \( \xi \) ranges where \( D(\xi) > 2 \) are band gaps at \( k = 0 \). Two linearly independent solutions of the Eq. (A.4) can be written in the form of (A.16) \((\beta > 0)\): \( y(\xi, \pm \beta, x + a) = e^{\pm \beta a} y(\xi, \pm \beta, x) \) where \( \beta \) and \( \xi \) are related by (A.17). By using \( x = -\frac{a}{2} \) in (A.16) and writing \( y(\xi, \pm \beta, x) \) in the form (A.20) with Eq. (A.10) we obtain that

\[
\frac{c_2}{c_1} = \pm \frac{\xi}{a} \cos \frac{\xi}{2} \sqrt{\frac{D - 2}{D + 2}},
\]

where \( D = 2 \cos \xi + 2p \frac{\xi}{2} \sin \xi \) is the discriminant of (A.4). Since \( D > 2 \) for a \( \xi \) inside a band gap at \( k = 0 \), we have

\[
y(\xi, \pm \beta, x) = C \left[ \sin \frac{\xi}{2} \sqrt{D + 2} \eta_1(x, \xi) \pm \frac{\xi}{a} \cos \frac{\xi}{2} \sqrt{D - 2} \eta_2(x, \xi) \right], \quad (A.32)
\]

where \( C \) is a normalized constant. We choose the normalization constant \( C \) in Eq. (A.32) similarly as in Sect. A.3.3.1. Thus

\[
y(\xi, \pm \beta, x) = \begin{cases} 
\frac{2}{\sin \xi (\sqrt{D + 2} + \sqrt{D - 2})} \left[ \sin \frac{\xi}{2} \sqrt{D + 2} \cos \left( \frac{\xi}{2} + \frac{\xi}{a} x \right) \right. \\
\pm \cos \frac{\xi}{2} \sqrt{D - 2} \sin \left( \frac{\xi}{2} + \frac{\xi}{a} x \right) , & -\frac{a}{2} \leq x \leq 0, \\
\frac{2}{\sin \xi (\sqrt{D + 2} - \sqrt{D - 2})} \left[ \sin \frac{\xi}{2} \sqrt{D + 2} \cos \left( \frac{\xi}{2} - \frac{\xi}{a} x \right) \right. \\
\mp \cos \frac{\xi}{2} \sqrt{D - 2} \sin \left( \frac{\xi}{2} - \frac{\xi}{a} x \right) , & 0 \leq x \leq \frac{a}{2},
\end{cases} \quad (A.33)
\]

by requiring \( y(\xi, \pm \beta, 0) = 1 \). The first part of Eq. (A.33) is directly from Eqs. (A.32) and (A.10), the second part comes from that due to the inversion symmetry of Eq. (A.4), \( y(\xi, +\beta, x) \) in the +\( x \) direction behaves exactly same as \( y(\xi, -\beta, x) \) in the -\( x \) direction: \( y(\xi, \pm \beta, x) = y(\xi, \mp \beta, -x) \).

In Figs. A.5 and A.6 are shown the functions \( y(\xi, \beta, x) \) and \( y(\xi, -\beta, x) \) of two different \( \xi \) in the lowest band gap at \( k = 0 \).

Zeros of Solutions:

The zeros \( x_0 \) of a solution \( y(\xi, \pm \beta, x) \) in (A.33) of Eq. (A.4) for \( \xi \) in a band gap at \( k = 0 \) is determined by

\[
y(\xi, \pm \beta, x_0) = 0.
\]

Thus the zeros \( x = x_0 \) of \( y(\xi, \pm \beta, x) \) are the solutions of one of the following two equations:

\[
cot \left( \frac{\xi}{2} + \frac{\xi}{a} x_0 \right) = \mp \sqrt{\frac{-\sin \xi + \xi (1 + \cos \xi)}{\sin \xi + \xi (1 - \cos \xi)}}, \quad -\frac{a}{2} \leq x_0 \leq 0
\]

\[
cot \left( \frac{\xi}{2} - \frac{\xi}{a} x_0 \right) = \pm \sqrt{\frac{-\sin \xi + \xi (1 + \cos \xi)}{\sin \xi + \xi (1 - \cos \xi)}}, \quad 0 \leq x_0 \leq \frac{a}{2}
\]

(A.34)
Fig. A.5 The functions $y(ξ, β, x)$ (A.33) with two different energies in the lowest band gap at $k = 0$. Note the discontinuity of the derivatives of the functions at $x = 0$ due to (A.7). Note that each function has two zeros in the interval $(-\frac{a}{2}, \frac{a}{2})$ and the zeros of the functions go left from the zeros of $φ_1(0, x)$ (solid circles) to the zeros of $φ_2(0, x)$ (open circles) as $ξ$ increases.

Fig. A.6 The functions $y(ξ, -β, x)$ (A.33) with two different energies in the lowest band gap at $k = 0$. Note the discontinuity of the derivatives of the functions at $x = 0$ due to (A.7). Note that each function has two zeros in the interval $(-\frac{a}{2}, \frac{a}{2})$ and the zeros of the functions go right from the zeros of $φ_1(0, x)$ (solid circles) to the zeros of $φ_2(0, x)$ (open circles) as $ξ$ increases.
The zeros \( x_0 \) of functions \( y(\xi, \beta, x) \) in the lowest band gap at \( k = 0 \) calculated by (A.34) for different \( \xi \) in the lowest band gap at the center of the Brillouin zone \( k = 0 \) are shown in Fig. A.7 as dashed lines. There are two zeros of \( y(\xi, \beta, x) \) in the interval \((-\frac{a}{2}, \frac{a}{2})\), as indicated by Theorem 2.8; As \( \xi \) increases from the lower edge \( \xi = \omega_1 \) to the upper edge \( \xi = \Omega_1 \), the zeros \( x_0 \) of \( y(\xi, \beta, x) \) go left from the zeros of \( \phi_1(0, x) \) (solid circles) to the zeros of \( \phi_2(0, x) \) (open circles).

The zeros \( x_0 \) of \( y(\xi, -\beta, x) \) calculated by Eq. (A.34) for different \( \xi \) in the lowest band gap at the center of the Brillouin zone \( k = 0 \) are shown in Fig. A.8 as double-dotted chained lines. There are two zeros of \( y(\xi, -\beta, x) \) in the interval \((-\frac{a}{2}, \frac{a}{2})\), as indicated by Theorem 2.8. As \( \xi \) increases from the lower edge \( \xi = \omega_1 \) to the upper edge \( \xi = \Omega_1 \), the zeros of \( y(\xi, -\beta, x) \) go right from the zeros of \( \phi_1(0, x) \) (solid circles) to the zeros of \( \phi_2(0, x) \) (open circles).

Figures A.7 and A.8 can be compared with Figs. 3.1 and 3.2 in Chap. 3.
A.4 Surface States in A Semi-infinite Kronig–Penney Crystal

For a one-dimensional semi-infinite Kronig–Penney crystal with a potential barrier at the left boundary at $\tau$, the problem can be written as

$$
-\psi''(x) + \left[ \sum_{n=-\infty}^{\infty} \frac{2p}{a} \delta(x-na) - \frac{\xi^2}{a^2} \right] \psi(x) = 0, \quad \tau < x < +\infty \tag{A.35}
$$

inside the crystal and a boundary condition at $\tau$:

$$
\psi'(\tau, \xi) - \sigma \psi(\tau, \xi) = 0, \tag{A.36}
$$

where $\sigma$ is a positive number depending on the potential barrier $U_{out}(x)$. Although $U_{out}(x)$ may have different forms, the effect of different $U_{out}(x)$ on the problem treated here can be simplified to the effect of $\sigma$. In the simplest cases, the potential outside the crystal is a constant $U_{out} = U_0$. We will only need to consider the cases where $-\frac{a}{2} \leq \tau \leq 0$.

A.4.1 Surface State Solutions

We will be only interested in the surface state solutions of Eqs. (A.35) and (A.36). We may use a similar approach as we used in Sect. A.3 to obtain such solutions. Nevertheless, the Kronig–Penney model is one of the cases where $\eta_1(\tau + a)$ and $\eta'_1(\tau + a)$ in Eqs. (3.18) and (3.19) can be analytically obtained. An even more convenient way is to use the formalism presented in Sect. 3.5 to investigate the existence and properties of surface states in a one-dimensional semi-infinite Kronig–Penney crystal.

From now on the two normalized solutions $\eta_1(x, \xi)$ and $\eta_2(x, \xi)$ of Eq. (A.4) are defined by the conditions (3.14):

$$
\eta_1(\tau, \xi) = 1, \quad \eta'_1(\tau, \xi) = 0; \quad \eta_2(\tau, \xi) = 0, \quad \eta'_2(\tau, \xi) = 1. \tag{A.37}
$$

We can consider that a unit cell of the Kronig–Penney crystal described by Eqs. (A.1) and (A.2) is composed of three regions: a region of width $d_2$ with a potential $U_2$ between a region of width $d_1$ on the left and a region of width $d_3$ on the right, both with a zero potential. Here

$$
d_1 = -\tau, \quad d_3 = a + \tau, \quad -\frac{a}{2} \leq \tau \leq 0, \\
d_1 = a - \tau, \quad d_3 = \tau, \quad 0 \leq \tau \leq \frac{a}{2}. \tag{A.38}
$$
Appendix A: The Kronig–Penney Model

In the Kronig–Penney limit

\[ \lim d_2 = 0, \quad \lim (d_1 + d_3) = a, \quad \lim U_2d_2 = p. \]

For such a Kronig–Penney crystal Eqs. (C.33), (C.35) and (C.36) in Appendix C give that

\[
\begin{align*}
\eta_1(\tau + a, \xi) &= \cos \xi + 2p \xi c_{11}s_{33}, \\
\eta_2(\tau + a, \xi) &= \frac{p}{\xi}(\sin \xi + 2p \xi s_{11}s_{33}), \\
\eta_2'(\tau + a, \xi) &= \cos \xi + 2p \xi s_{11}c_{33},
\end{align*}
\]  

(A.39)

where \( c_{ll} = \cos kld_l, s_{ll} = \sin kld_l \) as defined in (C.11), and \( k_1 = k_3 = \frac{\xi}{a} \). Note from Eq. (A.39) the discriminant \( D(\xi) \) of such a Kronig–Penney crystal is

\[ D(\xi) = \eta_1(\tau + a, \xi) + \eta_2'(\tau + a, \xi) = 2(\cos \xi + \frac{p}{\xi}\sin \xi), \]

since \( d_1 + d_3 = a \). This is same as \( D(\xi) \) in (A.11).

From Eqs. (3.16) and (3.17) the existence of a surface state in a band gap is determined by

\[
\sigma a = \frac{p \sin \frac{\xi}{a}(d_1 - d_3) + \frac{\xi}{2}\sqrt{D^2(\xi) - 4}}{\sin \xi + \frac{p}{\xi}[\cos \frac{\xi}{a}(d_1 - d_3) - \cos \xi]} \quad (A.40)
\]

for a band gap at the Brillouin zone boundary \( k = \pi/a \); or

\[
\sigma a = \frac{p \sin \frac{\xi}{a}(d_1 - d_3) - \frac{\xi}{2}\sqrt{D^2(\xi) - 4}}{\sin \xi + \frac{p}{\xi}[\cos \frac{\xi}{a}(d_1 - d_3) - \cos \xi]} \quad (A.41)
\]

for a band gap at the Brillouin zone center \( k = 0 \). In (A.40) and (A.41), \( d_1 \) and \( d_3 \) are related to \( \tau \) by (A.38). These two equations determine the existence of surface states in band gaps and their properties, such as how the eigenvalue \( \Lambda = \xi^2/(\chi a)^2 \) of each existed surface state depends on \( \tau \) and \( \sigma \).

For cases where the outside potential barrier is a constant \( U_0 = q^2 \) [2, 7], we have that

\[ \sigma a = \sqrt{q^2 - \xi^2}. \quad (A.42) \]

In Fig. A.9 are shown the numerical results of the \( \tau - \xi \) relationships for four different \( U_0 = q^2 \) calculated by (A.41) and (A.42), for the lowest band gap at the Brillouin zone center \( k = 0 \). From this figure, we can see the following: First, for each specific outside barrier potential, there are \( \tau \) intervals in \( [-\frac{\xi}{2}, \frac{\xi}{2}] \), no \( \tau - \xi \) curves exist. That indicates that no surface state could exist in the band gap for the specific outside potential barrier \( U_0 = q^2 \) and a \( \tau \) in those intervals; Second, those no-surface state
Fig. A.9 The functions $\tau - \xi$ obtained from (A.41) and (A.42) with four different constant barrier potentials $q^2$ outside the semi-infinite Kronig–Penney crystal in the lowest band gap at $k = 0$. The double-dotted chain lines corresponding to $q = \infty$ are exact the same as the double-dotted chained lines in Fig. A.8. The other chained lines of different thickness correspond to that $q = 10\pi$ (thickest lines), $q = 5\pi$ and $q = 3\pi$ (thinnest lines).

Intervals move right as the outside barrier potential $q^2$ decreases, as analyzed in Chap. 3; Third, for a specific boundary $\tau$, the energy $\Lambda = \xi^2/(\chi a)^2$ of an existing surface state increases as the outside barrier potential $q^2$ increases, in consistence with Eq. (3.7); Fourth, for a specific outside barrier potential $q^2$, the energy of an existing surface state increases as $\tau$ increases, in consistence with Eq. (3.8).

In an ideal semi-infinite Kronig–Penney crystal where the boundary condition (A.36) at $\tau$ is simplified to

$$\psi(\tau, \xi) = 0.$$  \hfill (A.43)

A necessary condition for existence of a surface state now is

$$\psi(\tau + a, \xi) = \psi(\tau, \xi) = 0,$$  \hfill (A.44)

or simpler as

$$\eta_2(\tau + a, \xi) = 0,$$  \hfill (A.45)

from (A.37) or (3.21).
A.4.2 Comparisons with the Tamm’s Work and the Seitz’s Book

As an application of Eqs. (A.40) and (A.41), we compare the results obtained here with the results obtained in the Tamm’s classical work [5] and described in the Seitz’s classical book [2]. In Tamm’s work, a specific boundary location was used, that corresponds to \( \tau \to +0 \) in our more general investigation presented here.

In the limit \( \tau \to +0 \), both Eqs. (A.40) and (A.41) give

\[
\frac{p - \sigma a}{\xi} = \sqrt{\frac{p^2}{\xi^2} + 2 \frac{p}{\xi} \cot \xi - 1},
\]

(A.46)

since \( \sin \xi \geq 0 \) for a band gap at \( k = 0 \) and \( \sin \xi \leq 0 \) for a band gap at \( k = \pi/a \).

That is

\[
\sqrt{\frac{p^2}{\xi^2} + 2 \frac{p}{\xi} \cot \xi - 1} = \frac{p - \sqrt{q^2 - \xi^2}}{\xi}
\]

(A.47)

from (A.42). By squaring both sides of (A.47), we obtain that

\[
\frac{p^2}{\xi^2} + 2 \frac{p}{\xi} \cot \xi - 1 = \frac{(q^2 - \xi^2)^2 - 2p\sqrt{q^2 - \xi^2} + p^2}{\xi^2}
\]

and thus

\[
\xi \cot \xi = \frac{q^2}{2p} - \sqrt{q^2 - \xi^2}.
\]

(A.48)

This is Eq. (19) in Tamm’s paper [5]. It is also Eq. (3.18) in [7] and corresponds to Eq. (6) in p. 322 in Seitz’s book [2]. Equation (A.48) has one solution for each interval \( (n + 1)\pi < \xi < (n + 2)\pi \) if \( \sigma > 0 \), i.e., \( q^2 - \xi^2 > 0 \). Probably it was this fact that leads to a widely and long-time belief in the solid state physics community that there is always a surface state in each band gap below the barrier height due to the termination of the periodic potential [2]. Nevertheless, as Tamm pointed out [5] that the condition \( p - \sqrt{q^2 - \xi^2} > 0 \) is necessary since the left side of (A.47) is positive. Consequently, the number of solutions of (A.47) might be significantly less than the number of solutions of (A.48): A termination of the periodic potential at the boundary of a semi-infinite Kronig–Penney crystal may or may not cause a surface state in a specific band gap below the barrier height. The widespread and long-time belief that it always does, is a misunderstanding. It might be this belief that leads to another widely accepted belief that the two terminations of the periodic potential in a simple one-dimensional crystal of finite length cause two surface states - each being associated with either end of the finite crystal - in each band gap below the barrier height.
We can further demonstrate that the number of solutions of Eq. (A.47)—that is, the solutions in the Tamm’s original paper [5]—is limited, and sometimes the surface state solutions in the Tamm’s original paper actually may not exist at all.

The condition $p - \sqrt{q^2 - \xi^2} > 0$ and that $\sigma > 0$ in (A.42) lead to that if a surface state - a solution of (A.47) - can exist in a band gap, the following condition must be satisfied:

$$\sqrt{q^2 - p^2} < \xi < q. \quad (A.49)$$

To understand the problem more specifically, we discuss the case where the outside barrier has a specific $q$. In Fig. A.10 is shown that Fig. A.1 is combined with the condition (A.49) for a specific $q = 5\pi$. There are always four band gaps ($n = 0, 1, 2, 3$) below the barrier; each gap may have a solution satisfying (A.48). Nevertheless, whether and how many surface state solutions can exist in these four band gaps might be quite different for different Kronig–Penney crystals.

For a Kronig–Penney crystal of $p = 3\pi/2$, we see that all the four band gaps are below the dashed line, and thus, the condition (A.49) cannot be satisfied. Accordingly, in none of the four band gaps can there be a solution satisfying (A.47) and thus a surface state, although each gap may have a solution satisfying (A.48).

However, for a Kronig–Penney crystal of $p = 4\pi$, two band gaps ($n = 0, 1$) are below the dashed line and thus (A.49) cannot be satisfied. In none of the two band gaps can there be a solution satisfying (A.47) and thus a surface state; The other
two band gaps \( (n = 2, 3) \) are above the dashed line, thus (A.49) can be satisfied. Correspondingly, this Kronig–Penney crystal may have a surface state solution in each one of the two band gaps.

For a Kronig–Penney crystal of \( p = 4.95\pi \), all four band gaps are above the dashed line and thus (A.49) can be satisfied. Such a Kronig–Penney crystal may have a surface state solution in each one of the four band gaps below \( q = 5\pi \).

### A.5 Electronic States in A Finite Kronig–Penney Crystal of Length \( L = Na \)

For an ideal finite Kronig–Penney crystal of length \( L = Na \)—where \( N \) is a positive integer—with a left boundary at \( \tau \) thus a right boundary at \( \tau + L \), the electronic states are the solutions of the equation

\[
-\psi''(x) + \left[ \sum_{n=-\infty}^{\infty} \frac{2p}{a} \delta(x - na) - \frac{\xi^2}{a^2} \right] \psi(x) = 0, \quad \tau < x < \tau + L, \tag{A.50}
\]

with boundary conditions at \( \tau \) and \( \tau + L \) for an ideal crystal of finite length:

\[
\psi(\tau) = \psi(\tau + L) = 0. \tag{A.51}
\]

In general, a nontrivial solution of (A.50) with the boundary condition (A.51)—if it exists—can be expressed as

\[
\psi(\xi, x) = \begin{cases} y(\xi, x), & \tau < x < \tau + L, \\ 0, & x \leq \tau \text{ or } x \geq \tau + L, \end{cases}
\]

where \( y(\xi, x) \) is a linearly combination of the two independent solutions \( y_1(\xi, x) \) and \( y_2(\xi, x) \) of (A.4):

\[
y(\xi, x) = c_1 y_1(\xi, x) + c_2 y_2(\xi, x). \tag{A.52}
\]

\( y_1(\xi, x) \) and \( y_2(\xi, x) \) are determined by the discriminant \( D(\xi) \) of Eq. (A.4). \( y(\xi, x) \) in (A.52) is a general form of nontrivial solutions of Eq. (A.50). It is required to further satisfy

\[
y(\xi, \tau) = y(\xi, \tau + L) = 0. \tag{A.53}
\]

to give nontrivial solutions of (A.50) and (A.51).

We consider two different cases: (1) \( \xi \) is inside a permitted band and (2) \( \xi \) is not inside a permitted band. Without losing generality, we only need to consider \( \tau \) in one period \([\frac{-a}{2}, \frac{a}{2}]\).
A.5.1 \( \xi \) Is Inside a Permitted Band

If \( \xi \) is inside a permitted band of Eq. (A.4), two independent solutions \( y_1(\xi, x) \) and \( y_2(\xi, x) \) in (A.52) are two Bloch wave solutions \( \phi_n(\pm k, x) \) \((0 < k < \pi/a)\) given by (A.12):

\[
y_1(\xi, x) = \phi_n(k, x), \quad y_2(\xi, x) = \phi_n(-k, x).
\]

Equations (A.52) and (A.53) from Eq. (A.12) give that

\[
c_1 \phi_n(k, \tau) + c_2 \phi_n(-k, \tau) = 0, \quad -\frac{a}{2} \leq \tau \leq \frac{a}{2},
\]

(A.54)

Since neither \( \phi_n(k, \tau) \) nor \( \phi_n(-k, \tau) \) can be zero (Sect. A.3.1), from (A.54) we obtained that

\[
e^{ikL} - e^{-ikL} = 0
\]

(A.55)

is the condition that Eqs. (A.52) and (A.53) could have non-trivial solutions. Equation (A.55) has \( N - 1 \) solutions for \( 0 < k < \pi/a \):

\[
k = \frac{j\pi}{L}, \quad j = 1, 2, \ldots, N - 1.
\]

(A.56)

Thus, (A.50) and (A.51) has \( N - 1 \) solutions in each permitted band, with \( \xi \) determined by:

\[
\cos \frac{j\pi}{N} = \cos \xi + \frac{p}{\xi} \sin \xi, \quad j = 1, 2, \ldots, N - 1.
\]

(A.57)

A.5.2 \( \xi \) Is Not Inside a Permitted Band

\( \xi \) can be either inside a band gap or at a band edge if it is not inside a permitted band of Eq. (A.4).

If \( \xi \) is inside a band gap, two independent solutions \( y_1(\xi, x) \) and \( y_2(\xi, x) \) of (A.4) in (A.52) can be written either as the forms of (A.14) if the band gap is at \( k = \pi/a \) or as the forms of (A.16) if the band gap is at \( k = 0 \). By using a similar approach as we used to obtain (A.55), we obtain that

\[
y(\tau + a, \xi) = y(\tau, \xi) = 0
\]

(A.58)

is a necessary condition for the existence of solutions of (A.50) and (A.51).
Fig. A.11 The $\tau$-dependence of the solution $\xi$ of (A.50) and (A.51) in the lowest band gap at $k = 0$ for a Kronig–Penney crystal with $p = 3/2\pi$. For each $-\frac{a}{2} \leq \tau \leq \frac{a}{2}$, there is always one and only one solution $\xi$ of (A.50) and (A.51) in the band-gap, its corresponding $\psi$ is either a surface state located near the left end of the finite crystal (chained lines), or a surface state located near the right end of the finite crystal (dashed lines), or a confined band-edge state (solid circles and open circles).

If $\xi$ is at a band edge, we can choose $y_1(\xi, x)$ in (A.52) as a band-edge function described in Sect. A.3.2 and $y_2(\xi, x)$ as the other solution of (A.4) independent of $y_1(\xi, x)$. Based on the periodicity or semi-periodicity of the band-edge functions and the Sturm Separation Theorem, we know that only the band-edge function $y_1(\xi, x)$ can be a solution of (A.50) and (A.51) for $\xi$ at a band edge of Eq. (A.4). We also obtain that (A.58) is a necessary condition for the existence of solutions of (A.50) and (A.51).

From (A.58) we can obtain that

$$y(\tau + \ell a, \xi) = y(\tau, \xi) = 0,$$  \hspace{1cm} (A.59)

where $\ell = 1, 2, \ldots, N$. Therefore (A.58) is a necessary and sufficient condition for the existence of a solution of (A.50) with the boundary conditions (A.51) where $\xi$ is not inside a permitted band. Theorem 2.8 indicates that corresponding to each band gap, there is always one and only one solution of (A.58).

The calculated $P = \frac{y(\tau + a, \xi)}{y(\tau, \xi)} = \frac{y'(\tau + a, \xi)}{y'(\tau, \xi)}$ from (A.58) can have three possibilities: (a) $0 < |P| < 1$; (b) $|P| = 1$; (c) $|P| > 1$. The case (a) corresponds to a solution $\psi(x, \xi)$ of Eqs. (A.50) and (A.51) oscillatory decreasing in the $+x$ direction, indicating a surface state localized near the left boundary $\tau$; The case (b) corresponds to that $\psi(x, \xi)$ is a band-edge state of Eq. (A.4) in the finite crystal; The case (c) corresponds to an oscillatory increasing $\psi(x, \xi)$ in the $+x$ direction, thus an oscillatory decaying solution in the $-x$ direction, indicating a surface state localized near the right boundary $\tau + L$. 
As an example, in Fig. A.11 is shown the solution \( \xi \) of (A.50) and (A.51) in the lowest band gap at \( k = 0 \) for a Kronig–Penney crystal with \( p = 3/2\pi \). For each \(-\frac{a}{2} \leq \tau \leq \frac{a}{2}\), there is always one and only one \( \xi \) located in either one dashed line area or one chained line area, or at one circle. It corresponds to one solution \( \psi \) of (A.50) and (A.51) in the band-gap with a zero at \( \tau \) and \( \tau + L \), having the form of \( c_1 e^{\beta x} p_1(\xi, x) \) or \( c_2 e^{-\beta x} p_2(\xi, x) \), or being a periodic function. Such a solution indicates a surface state located near the right or the left end of the finite crystal, or, a confined band edge state. Figure A.11 is simply the combination of Figs. A.7 and A.8.

Therefore, all electronic states in an ideal Kronig–Penney crystal of finite length \( L = Na \)—including how the energy and wavefunction of each state depend on the parameter \( p \), the crystal boundary \( \tau \), and the crystal length \( L \)—can be analytically obtained. It is well-known that the Kronig–Penney model plays a significant role in our current understanding of electronic states in one-dimensional crystals with translational invariance. We have seen here that the model again provides a significant and analytical understanding of electronic states in an ideal one-dimensional periodic system of finite size.

References

5. I. Tamm: Phys. Z. Sowj. 1, 733 (1932)
Appendix B
Electronic States in One-Dimensional Symmetric Finite Crystals with a Finite $V_{out}$

The Schrödinger differential equation for a one-dimensional crystal can be written as

$$-y''(x) + [v(x) - \lambda]y(x) = 0.$$  \hfill (B.1)

Here, $v(x) = v(x+a)$ is the periodic potential of the crystal.

For a one-dimensional crystal of finite length $L = Na$, the eigenvalues $\Lambda$ and eigenfunctions $\psi(x)$ are solutions of the equation

$$-\psi''(x) + [v(x) - \Lambda]\psi(x) = 0, \quad \tau < x < \tau + L,$$  \hfill (B.2)

inside the crystal with certain boundary conditions at the two boundaries $\tau$ and $\tau + L$.

If the potential outside the crystal $V_{out} = +\infty$, we have the boundary conditions

$$\psi(x) = 0, \quad x = \tau \text{ or } x = \tau + L.$$  \hfill (B.3)

This is the case treated in Chap. 4. It is found that for each band gap, there is always one and only one state whose energy is boundary dependent but independent of the crystal length. A surface state is one of the two possibilities of such a boundary-dependent state. Therefore, there is at most one surface state in each band gap in an ideal one-dimensional finite crystal.

Many years ago, Shockley published a classic paper [1]. The paper stated that in a one-dimensional symmetric finite crystal when the potential period $a$ is so small that the boundary curves for allowed energy bands have crossed, and the number of atoms $N$ in the crystal is very large, the surface states appear in pairs in band gaps. To clearly understand the relationship between the results of [1] and Chap. 4, in this Appendix we investigate the cases where the electrons are not completely confined to the crystal as in [1], and the crystal length may not be very long.

Now, we need to consider the cases where $V_{out}$ is finite. Qualitatively, the effect of a finite $V_{out}$ can be directly obtained from a theorem in [2]: A finite $V_{out}$ moves all energy levels lower. Quantitatively, a finite $V_{out}$ will allow a small part of the electronic state spills out of the finite crystal and thus, make the boundary conditions be
\[
\frac{\psi' / \psi}{x=\tau} = \sigma_1, \\
\frac{\psi' / \psi}{x=\tau+L} = -\sigma_2, \tag{B.4}
\]

instead of (B.3). Here, \(\sigma_1\) and \(\sigma_2\) are positive numbers depending on \(V_{out}\). Note that (B.3) corresponds to \(\sigma_1 = \sigma_2 = +\infty\), and \(\sigma_1\) and \(\sigma_2\) will monotonically decrease as \(V_{out}\) decreases. Although \(V_{out}\) may have different forms, the effect of different \(V_{out}\) to the problem treated here can be simplified to be the effect of \(\sigma_1\) and \(\sigma_2\).

Shockley treated one-dimensional symmetric finite crystals with finite \(V_{out}\), where \(\sigma_1 = \sigma_2 = \sigma\). His treatment provided a way to investigate how much the results obtained in Chap. 4 are dependent on \(V_{out}\) for symmetric one-dimensional finite crystals. For the convenience of comparison with his original paper, we use his approach assuming that the cell potential in the crystal is symmetric and use same notations as in [1] except that the energy is written as \(\lambda\) rather than \(E\) and the number of atoms in the crystal is \(N\) in this appendix. As in Shockley’s paper, we also consider the two lowest band gaps: one at \(k = \pi/a\) and one at \(k = 0\).

Assuming \(g(x)\) and \(u(x)\) are two linearly independent solutions of the Schrödinger differential equation (B.1) in a unit cell, symmetric or antisymmetric to the cell center \(x = 0\), Shockley obtained \(g(a/2)u'(a/2)(1 - e^{-ika}) = g'(a/2)u(a/2)(1 + e^{ika})\) and further that \(\sigma = \mu \tan(ka/2) \tan(Nka/2)\) and \(\sigma = -\mu \tan(ka/2) \cot(Nka/2)\) (Eqs. (11) and (12) in [1]) give the energies of electronic states in the one-dimensional finite crystal; here, \(\mu = u'(a/2)u(a/2)/a\). Therefore, the effect of finite \(V_{out}\) can be found from the \(\sigma\) dependence of energy levels. In Fig. B.1 is shown a numerical calculation for the electronic states near the upper band-edge \(\varepsilon_2(0)\) of the band gap at \(k = 0\) in crystals of two different lengths, \(N = 14\) and \(N = 15\), with a model cell potential \(v(x) = -30\) if \(|x| \leq 0.38\) and \(v(x) = 0\) if \(0.38 < |x| \leq 0.5\) and \(a = 1\). It can be seen that lowering \(V_{out}\) (thus lowering \(\sigma\)) moves all energy levels downward. However, the energy of the state in the band gap depends on the crystal length much less than the states in the energy band: The major difference between the state corresponding to a band gap and the states corresponding to an energy band obtained in Sect. 4.2 remains.

For many physical situations, \(\sigma\) can be considered as sufficiently large [3]. It can be shown that for those states in Fig. B.1, in the limit of large \(\sigma\) (i.e., large \(V_{out}\)), the energies of the states in the energy band can approximately be given by

\[
\Lambda_{2,j} = \varepsilon_2(k_j)
\]

and

\[
k_j = \frac{j\pi}{Na} - \frac{2}{Na} \frac{\mu}{\sigma} \tan\left(\frac{j\pi}{2N}\right), \quad j = 1, 2, \ldots, N - 1, \tag{B.5}
\]

where \(\mu > 0\). On the other hand, the energy of the state in the gap is given approximately by \((\varepsilon_2''(0) > 0)\).
\[ \sigma = \mu \tan \left( \frac{ka}{2} \right) \tan \left( \frac{Nka}{2} \right) \]

\[ \text{and} \]

\[ \sigma = -\mu \tan \left( \frac{ka}{2} \right) \cot \left( \frac{Nka}{2} \right) \]

calculated for \( N = 14 \) (solid lines) and \( N = 15 \) (long dashed lines) near the upper band edge \( \varepsilon_2(0) \) of the band gap at \( k = 0 \). The short-dashed vertical line is the band edge. Note the energy of the state in the band gap almost does not depend on the crystal length, even for a finite \( \sigma \).

\[ \Lambda_{1,\text{gap}} = \varepsilon_2(0) - \varepsilon''_2(0) \frac{6(c - 1)}{(cN^2 - 1)a^2}; \]

here, \( c = -\sigma N/\mu > 1, \mu < 0 \), and \( c \to 1 \) when \( \sigma \to +\infty \). Again, it can be clearly seen that lowering \( \sigma \) (lowering \( V_{\text{out}} \)) moves all energy levels downward, and the energy of the state in the band gap depends on the crystal length much less than the energies of the states in the energy band.

Shockley found that when (i) the potential period \( a \) is so small that the boundary curves for allowed energy bands have crossed and (ii) the number of atoms in the crystal \( N \) is very large, the surface states appear in pairs in the band gap. Now, we try to give this problem a more careful investigation and attempt to understand whether and how “two surface states” in a band gap could happen in a one-dimensional symmetric finite crystal. We also consider the cases of \( N \) is even, as in [1].

In general, inside a band gap, an electronic state as a nontrivial solution of (B.1) always has the form

\[ y(x) = Ae^{\beta x} f_1(x) + Be^{-\beta x} f_2(x) \]  \hspace{1cm} (B.6)

from (2.77) or (2.81); here, \( A \) and \( B \) are not both zero, \( \beta > 0 \), and \( f_i(x) \) is either a periodic function \( (f_i(x + a) = f_i(x)) \) if the band gap is at \( k = 0 \) or a semi-periodic function \( (f_i(x + a) = -f_i(x)) \) if the band gap is at \( k = \pi/a \). Equation (B.6) is more general than the simple surface states in which either \( A \) or \( B \) is zero thus the state is localized near one end of the crystal. Such a state (B.6) in a symmetric one-dimensional finite crystal must be either symmetric \( (A = B) \) or antisymmetric \( (A = -B) \) and, thus, is equally localized near the both ends of the finite crystal and can be considered as a generalized surface state. We are trying to investigate how many states of type (B.6), as solutions of (B.2) with the boundary conditions (B.4), are in a specific band gap.

For the gap at \( k = \pi/a \), two band-edge states are given by either \( g(a/2) = 0 \) or \( u'(a/2) = 0 \), as in [1]. Both band-edge wavefunctions have one node in a unit
cell \([-a/2, a/2]\) (Theorem 2.7). One (given by \(g(a/2) = 0\)) is symmetric to the cell center and has its most electron density at the cell center and zero density at the cell boundaries. The other one (given by \(u'(a/2) = 0\)) is antisymmetric to the cell center and has its most electronic density at the cell boundaries \(x = \pm a/2\) and zero density at the cell center.

No matter how small \(a\) is, if the cell potential at the cell boundaries is higher than the potential at the cell center as shown in Fig. 1a in [1] and the form of the cell potential is reasonable and not very irregular; we expect that \(g(a/2) = 0\) gives the lower band-edge state and \(u'(a/2) = 0\) gives the higher band-edge state: A state with most of its electronic density in the potential valley should have lower energy than a state with most of its electronic density around the potential peak. As an example, this point can be seen in Fig. A.3 where the lower band-edge wavefunction \(\phi_0(\pi/a, x)\) is zero at the potential peak and has all electronic density in the potential valley.\(^1\) In fact, Levine [3] did not observe a band-crossing either. Shockley has shown that the two surface states in the gap can happen only when \(g(a/2) = 0\) gives the higher band-edge state. Thus, the existence of two surface states in the lowest gap at \(k = \pi/a\), as shown in Fig. 2 in [1], seems unlikely for a reasonably regular one-dimensional finite crystal. Consistent with the analysis here, many other authors did not obtain a “Shockley” surface state in the lowest gap at \(k = \pi/a\) either [3, 4].

Then we consider the next band gap at \(k = 0\). The two band-edge states are given by either \(g'(a/2) = 0\) or \(u(a/2) = 0\); which one is higher depends on the form of the cell potential. If \(V_{out} = +\infty\), equations (11) and (12) in [1] for \(\sigma = +\infty\) give \(N - 1\) states \((k_j = j\pi/Na, j = 1, 2, \ldots, N - 1)\) for each energy band and one confined band-edge state for each band gap. The confined band-edge state for this band gap is the band-edge state given by \(u(a/2) = 0\) since its wavefunction is zero at the crystal boundaries. These results are consistent with Sect. 4.4.

If the confined band-edge state is at the lower band-edge \(\varepsilon_1(0)\) when \(V_{out} = +\infty\), an (any) finite \(V_{out}\) will move it downward into the energy band \(\varepsilon_1(k)\) below and, thus, will not make a surface state. Only if the confined band-edge state is at the upper band-edge \(\varepsilon_2(0)\) when \(V_{out} = +\infty\), an (any) finite \(V_{out}\) will move it downward into the band gap and thus make a surface state. That corresponds to the case that \(u(a/2) = 0\) gives the higher band-edge state.

In Fig. B.2 is shown a numerical calculation of such a situation, using the same model cell potential as in Fig. B.1, in comparison with Fig. 4 in [1]. When \(V_{out} = +\infty(\sigma = +\infty), u(a/2) = 0\) gives an antisymmetric confined band-edge state at the upper band-edge \(\varepsilon_2(0)\). Any finite \(\sigma\) due to a finite \(V_{out}\) can move this state (long-dashed line) into the band gap and thus make one antisymmetric gap state. However, moving a symmetric state (solid line) crossing the higher band-edge \(\varepsilon_2(0)\) into the band gap and making another surface state requires

\[
\sigma < -N\gamma_u; \quad (B.7)
\]

\(^1\)Please be aware of that \(\pm a/2\) are at a potential peak in Shockley’s paper [1] whereas in a potential valley in Fig. A.3.
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Fig. B.2 $\gamma \times 100$ (dotted line), $\mu$ (chained line), $\mu \tan(ka/2) \tan(Nka/2)$ (solid line) and $-\mu \tan(ka/2) \cot(Nka/2)$ (long-dashed line) for $N = 14$ near the band gap at $k = 0$ where the surface state(s) may exist. The left short-dashed vertical line corresponds to the lower band edge $\varepsilon_{1}(0)$, and the right short-dashed vertical line corresponds to the upper band edge $\varepsilon_{2}(0)$ here, $\gamma_u$ is $\gamma (= g'(a/2)/g(a/2))$ at the upper band-edge, a negative number. Therefore, in principle, if there are two surface states (one antisymmetric and one symmetric) in the gap, $\sigma$ (or $V_{out}$) needs to be small, and $N$ needs to be large. However, a too small $\sigma$ (or $V_{out}$) may even move the antisymmetric surface state crossing the lower band edge $\varepsilon_{1}(0)$ out of the band gap and into the lower energy band $\varepsilon_{1}(k)$. This case happens when $\sigma < -\mu_l/N$; here, $\mu_l$ is $\mu$ at the lower band-edge $\varepsilon_{1}(0)$, also a negative number. Note that $\mu_l$ and $\gamma_u$ are determined by the cell potential, and $\sigma$ is dependent on $V_{out}$. Figure B.2 shows the case for $N = 14$: When a small enough $\sigma$ (or $V_{out}$) moves the symmetric state (solid line) from the upper band $\varepsilon_{2}(k)$ into the band gap, the antisymmetric surface state (long-dashed line) almost enters the lower band $\varepsilon_{1}(k)$. In fact, $\sigma$ usually is quite large [3]. Depending on $\sigma$ or $V_{out}$, usually a much larger $N$ is needed to satisfy $\sigma < -N \gamma_u$. An even greater $N$ is required if the two surface states are almost degenerated. Two degenerated gap states of (B.6) type—one symmetric and one antisymmetric in a symmetric one-dimensional finite crystal—can be linearly combined and transformed to two surface states, one at each end.

The analysis here, as in Shockley’s paper [1], are for symmetric one-dimensional finite crystals. Nevertheless, we can also obtain some understanding of the surface states in general one-dimensional finite crystals. Since there is only one state corresponding to each gap for general one-dimensional finite crystals when $V_{out} = +\infty$ and a finite $V_{out}$ always moves all energy levels downward, in any case, if there are two states in a specific band gap for a finite $V_{out}$, one state must come from the permitted band above that band gap and is driven downward by the finite $V_{out}$. This state had an energy $\varepsilon_{2m+2}(\pi/Na)$ (for a band gap at $k = 0$) or $\varepsilon_{2m+1}[(N-1)\pi/Na]$ (for a band gap at $k = \pi/a$) when $V_{out} = +\infty$, independent of whether the crystal is small; for example, see [5, 6]. Thus, from (B.5), one can obtain that usually $(2\mu/\sigma) \tan(j\pi/2N) << 1$.  

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2In almost all previously published numerical calculations, the deviations from $k_j=j\pi/(Na)$ is small; for example, see [5, 6]. Thus, from (B.5), one can obtain that usually $(2\mu/\sigma) \tan(j\pi/2N) << 1$.  

symmetric or not. Only a small enough $V_{out}$ (depending on $N$) can move it crossing the band-edge into the band gap. The smaller $N$ is, the further the state is to the upper band-edge $\varepsilon_{2m+2}(0)$ or $\varepsilon_{2m+1}(\pi/a)$, and the more difficult is the state to be moved into the band gap by a finite $V_{out}$. Therefore, we can expect that a not very long one-dimensional finite crystal has at most one gap state in each band gap. However, the localization of this gap state might be somewhat different for a nonsymmetric finite crystal: Because when $V_{out} = +\infty$, a gap state in a nonsymmetric finite crystal may have either $A = 0$ or $B = 0$ in (B.6) (i.e., the state could be localized near one end of the crystal), as $V_{out}$ decreases there seems no understandable reason for that the localization behavior of the gap state will have a dramatic change. Thus, we can expect that such a gap state might be mainly localized near one end of the nonsymmetric finite crystal.

References

1. W. Shockley, Phys. Rev. 56, 317 (1939)
2. R. Courant, D. Hilbert, Methods of Mathematical Physics, vol. 1, p. 409, (Interscience, New York, 1953) (Theorem 3 and the relevant footnote)
3. J.D. Levine, Phys. Rev. 171, 701 (1968)
Appendix C
Layered Crystals

A layered crystal discussed in this book refers to a specific kind of periodically layered structures, in which each period is composed of two or more layers of homogeneous isotropic media. The wave equation in such a crystal can generally be written as a Sturm–Liouville equation with periodic coefficients:

\[ [p(x)y'(x)]' + [\lambda w(x) - q(x)]y(x) = 0, \quad (C.1) \]

where \( p(x) > 0, \ w(x) > 0 \) and \( q(x) \) are real constants in each layer and are all periodic with the same period \( a \):

\[ p(x+a) = p(x), \quad q(x+a) = q(x), \quad w(x+a) = w(x). \quad (C.2) \]

Each period unit of the simplest layered crystals is usually composed of two different media [1–5]. However, in some cases one might also need to deal with layered crystals in which each period is composed of three or more layers of different media [6–9].

In this Appendix, we apply the theory of periodic Sturm–Liouville equations in Chap. 2 to treat layered crystals and to obtain some general expressions for later use. We consider an (any) specific period of a layered crystal which is composed of \( N \) layers of different homogeneous isotropic media. Each layer \( l \) has a layer thickness \( d_l \), where \( l = 1, 2, \ldots, N \). The two ends of the \( l \)th layer are denoted to be \( x_{l-1} \) and \( x_l \) thus \( d_l = x_l - x_{l-1} \). We choose \( x_0 = 0, \) thus \( x_N = a \) is the period of the layered crystal. Inside the \( l \)th layer

\[ p(x) = p_l, \quad q(x) = q_l, \quad w(x) = w_l, \quad (C.3) \]

are real constants and \( p_l > 0, \ w_l > 0 \). Equation \((C.1)\) in each layer now can be written in the form

\[ [p_l y'(x)]' + [\lambda w_l - q_l] y(x) = 0, \quad x_{l-1} \leq x \leq x_l. \quad (C.4) \]
Or equivalently

\[ [p_l y'(x)]' + p_l k_l^2 y(x) = 0, \quad x_{l-1} \leq x \leq x_l, \quad (C.5) \]

by introducing

\[ p_l k_l^2 = \lambda w_l - q_l, \quad (C.6) \]

\( k_l \) is real if \( \lambda w_l - q_l > 0 \) or imaginary if \( \lambda w_l - q_l < 0 \).

According to the theory in Chap. 2, the band structure of such a layered crystal is determined by the discriminant of the Eq. (C.1):

\[ D(\lambda) = \eta_1(a, \lambda) + p(a)\eta_2'(a, \lambda), \quad (C.7) \]

where \( \eta_1(x, \lambda) \) and \( \eta_2(x, \lambda) \) are two linearly independent normalized solutions of (C.1) that satisfy

\[ \eta_1(0, \lambda) = 1, \quad p(0)\eta_1'(0, \lambda) = 0; \quad \eta_2(0, \lambda) = 0, \quad p(0)\eta_2'(0, \lambda) = 1. \quad (C.8) \]

by (2.53).

From (C.5) we have in the \( l \)th layer

\[ \eta_1(x, \lambda) = A_l \cos k_l x + B_l \sin k_l x; \quad p(x)\eta_1'(x, \lambda) = -p_l k_l A_l \sin k_l x + p_l k_l B_l \cos k_l x, \quad x_{l-1} \leq x \leq x_l, \quad (C.9) \]

where \( k_l \) is determined by \( p_l, q_l, w_l \) and the eigenvalue \( \lambda \) from (C.6). By defining

\[ f_l = p_l k_l, \quad (C.10) \]

at \( x = x_{l-1} \) we have

\[ \eta_1(x_{l-1}, \lambda) = A_l \cos k_l x_{l-1} + B_l \sin k_l x_{l-1}; \quad p_{l-1} \eta_1'(x_{l-1}, \lambda) = -f_l A_l \sin k_l x_{l-1} + f_l B_l \cos k_l x_{l-1}. \]

\( A_l \) and \( B_l \) can be obtained as,

\[ A_l = \eta_1(x_{l-1}, \lambda) \cos k_l x_{l-1} - \frac{1}{f_l} p_{l-1} \eta_1'(x_{l-1}, \lambda) \sin k_l x_{l-1}, \]

\[ B_l = \eta_1(x_{l-1}, \lambda) \sin k_l x_{l-1} + \frac{1}{f_l} p_{l-1} \eta_1'(x_{l-1}, \lambda) \cos k_l x_{l-1}. \]

By writing

\[ c_{l l} = \cos k_l d_l, \quad s_{l l} = \sin k_l d_l \quad (C.11) \]
for brevity, at $x = x_l$ from (C.9) we obtain

$$\eta_1(x_l, \lambda) = \eta_1(x_{l-1}, \lambda) c_{ll} + \frac{1}{f_l} p_{l-1} \eta'_1(x_{l-1}, \lambda) s_{ll},$$

$$p_l \eta'_1(x_l, \lambda) = p_{l-1} \eta'_1(x_{l-1}, \lambda) c_{ll} - \frac{1}{f_l} \eta_1(x_{l-1}, \lambda) s_{ll}.$$

These two equations can be written as

$$\begin{pmatrix} \eta_1(x_l, \lambda) \\ p_l \eta'_1(x_l, \lambda) \end{pmatrix} = \begin{pmatrix} c_{ll} & \frac{1}{f_l} s_{ll} \\ -\frac{1}{f_l} s_{ll} & c_{ll} \end{pmatrix} \begin{pmatrix} \eta_1(x_{l-1}, \lambda) \\ p_{l-1} \eta'_1(x_{l-1}, \lambda) \end{pmatrix}. \quad (C.12)$$

Similarly, we have

$$\begin{pmatrix} \eta_2(x_l, \lambda) \\ p_l \eta'_2(x_l, \lambda) \end{pmatrix} = \begin{pmatrix} c_{ll} & \frac{1}{f_l} s_{ll} \\ -\frac{1}{f_l} s_{ll} & c_{ll} \end{pmatrix} \begin{pmatrix} \eta_2(x_{l-1}, \lambda) \\ p_{l-1} \eta'_2(x_{l-1}, \lambda) \end{pmatrix}. \quad (C.13)$$

Equations (C.12) and (C.13) can be further written as

$$\tilde{\eta}_l(x_l, \lambda) = M_l \tilde{\eta}_l(x_{l-1}, \lambda) = \prod_{j=l}^{1} M_j \tilde{\eta}_l(x_0, \lambda) = M_l \tilde{\eta}_l(x_0, \lambda), \quad i = 1, 2, \quad (C.14)$$

where

$$\tilde{\eta}_l(x_l, \lambda) = \begin{pmatrix} \eta_l(x_l, \lambda) \\ p_l \eta'_l(x_l, \lambda) \end{pmatrix}, \quad l = 1, \ldots, N, \quad (C.15)$$

and

$$M_j = \begin{pmatrix} c_{jj} & \frac{1}{f_j} s_{jj} \\ -\frac{1}{f_j} s_{jj} & c_{jj} \end{pmatrix}, \quad j = 1, \ldots, N, \quad (C.16)$$

and

$$M_l = M_l M_{l-1} \cdots M_1 = \prod_{j=l}^{1} M_j. \quad (C.17)$$

By (C.8),

$$\tilde{\eta}_1(x_0, \lambda) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \tilde{\eta}_2(x_0, \lambda) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (C.18)$$
For a layered crystal composed of $N$ different homogeneous isotropic media, $x_N = a$. Equation (C.14) gives that

$$\eta_1(a, \lambda) = (M_N)_{11}, \quad (C.19)$$

$$p(a)\eta_1'(a, \lambda) = (M_N)_{21}; \quad (C.20)$$

and

$$\eta_2(a, \lambda) = (M_N)_{12}, \quad (C.21)$$

$$p(a)\eta_2'(a, \lambda) = (M_N)_{22}. \quad (C.22)$$

The discriminant $D(\lambda)$ of Eq. (C.1) is

$$D(\lambda) = \eta_1(a, \lambda) + p(a)\eta_2'(a, \lambda) = \text{Tr}(M_N). \quad (C.23)$$

The band structure of the eigen-modes is determined by

$$\cos ka = \frac{1}{2} D(\lambda) = \frac{1}{2} \text{Tr}(M_N), \quad (C.24)$$

where $-2 \leq D(\lambda) \leq 2$. Equations (C.19)–(C.24) and (C.16)–(C.17) are the basis of our treatments to layered crystals composed of different homogeneous and isotropic media, as in Appendices A, E and F.³

For $l = 1$, (C.19)–(C.22) give that

$$\eta_1(x_1, \lambda) = c_{11}, \quad p_1\eta_1'(x_1, \lambda) = -f_1 s_{11}, \quad (C.25)$$

$$\eta_2(x_1, \lambda) = \frac{1}{f_1} s_{11}, \quad p_1\eta_2'(x_1, \lambda) = c_{11}. \quad (C.26)$$

For a layered crystal composed of two different media, $N = 2$ and $x_2 = a$. (C.19)–(C.22) give that

$$\eta_1(a, \lambda) = c_{22}c_{11} - \frac{f_1}{f_2} s_{22}s_{11}, \quad (C.27)$$

$$p(a)\eta_1'(a, \lambda) = -f_1 c_{22}s_{11} - f_2 s_{22}c_{11}. \quad (C.28)$$

³Equations similar to (C.24), (C.17) and (C.16) were obtained as Eqs. (10), (11), (A.2) and (A.3) in [7]. The mathematical theory of periodic Sturm–Liouville equations straightforwardly gives more and general results. Equation (A.4) in [7] is simply a specific case of that the Wronskian of the solutions of a periodic Sturm–Liouville equation is a constant.
\[\eta_2(a, \lambda) = \frac{1}{f_1} c_{33}s_{22} + \frac{1}{f_2} s_{22}c_{11}, \quad (C.29)\]

and

\[p(a)\eta'_2(a, \lambda) = c_{22}c_{11} - \frac{f_2}{f_1} s_{22}s_{11}. \quad (C.30)\]

Equation (C.23) gives that

\[D(\lambda) = 2c_{22}c_{11} - \left(\frac{f_1}{f_2} + \frac{f_2}{f_1}\right) s_{22}s_{11}. \quad (C.31)\]

In the region \(-2 \leq D(\lambda) \leq 2\), the band structure can be more explicitly written as

\[\cos ka = \cos k_2d_2 \cos k_1d_1 - \frac{1}{2} \left(\frac{f_1}{f_2} + \frac{f_2}{f_1}\right) \sin k_2d_2 \sin k_1d_1 \quad (C.32)\]

by (C.24). This equation has been well known in the literature, see, for example, [1–5].

Further for a layered crystal of that each period is composed of three layers of different media, \(N = 3\) and \(x_3 = a\). Equations (C.19)–(C.22) give that

\[\eta_1(a, \lambda) = c_{33}c_{22}c_{11} - \frac{f_1}{f_2} c_{33}s_{22}s_{11} - \frac{f_1}{f_3} s_{33}c_{22}s_{11} - \frac{f_2}{f_3} s_{33}s_{22}c_{11}, \quad (C.33)\]

\[p(a)\eta'_1(a, \lambda) = -f_1 c_{33}c_{22}s_{11} - f_2 c_{33}s_{22}c_{11} - f_3 s_{33}c_{22}c_{11} + \frac{f_3}{f_2} s_{33}s_{22}s_{11}, \quad (C.34)\]

\[\eta_2(a, \lambda) = \frac{1}{f_1} c_{33}c_{22}s_{11} + \frac{1}{f_2} c_{33}s_{22}c_{11} + \frac{1}{f_3} s_{33}c_{22}c_{11} - \frac{f_2}{f_1f_3} s_{33}s_{22}s_{11}, \quad (C.35)\]

and

\[p(a)\eta'_2(a, \lambda) = c_{33}c_{22}c_{11} - \frac{f_2}{f_1} c_{33}s_{22}s_{11} - \frac{f_3}{f_1} s_{33}c_{22}s_{11} - \frac{f_3}{f_2} s_{33}s_{22}c_{11}. \quad (C.36)\]

Equation (C.23) gives that

\[D(\lambda) = 2c_{33}c_{22}c_{11} - \left(\frac{f_1}{f_2} + \frac{f_2}{f_1}\right) c_{33}s_{22}s_{11} - \left(\frac{f_1}{f_3} + \frac{f_3}{f_1}\right) s_{33}c_{22}s_{11}
- \left(\frac{f_2}{f_3} + \frac{f_3}{f_2}\right) s_{33}s_{22}c_{11}. \quad (C.37)\]
In the region $-2 \leq D(\lambda) \leq 2$, by Eq. (C.24) the band structure can be more explicitly written as

$$\cos ka = \cos k_3 d_3 \cos k_2 d_2 \cos k_1 d_1$$

$$-\frac{1}{2} \left( \frac{f_1}{f_2} + \frac{f_2}{f_1} \right) \cos k_3 d_3 \sin k_2 d_2 \sin k_1 d_1$$

$$-\frac{1}{2} \left( \frac{f_1}{f_3} + \frac{f_3}{f_1} \right) \sin k_3 d_3 \cos k_2 d_2 \sin k_1 d_1$$

$$-\frac{1}{2} \left( \frac{f_2}{f_3} + \frac{f_3}{f_2} \right) \sin k_3 d_3 \sin k_2 d_2 \cos k_1 d_1. \quad (C.38)$$

Further for a layered crystal in which each period is made of four layers of different homogeneous media, $N = 4$ and $x_4 = a$. Equations (C.19)–(C.22) give that

$$\eta_1(a, \lambda) = c_{44} c_{33} c_{22} c_{11} - \frac{f_1}{f_2} c_{44} c_{33} s_{22} s_{11} - \frac{f_1}{f_3} c_{44} s_{33} c_{22} s_{11}$$

$$-\frac{f_2}{f_3} c_{44} s_{33} s_{22} c_{11} - \frac{f_1}{f_4} s_{44} c_{33} c_{22} s_{11} - \frac{f_2}{f_4} s_{44} c_{33} s_{22} c_{11}$$

$$-\frac{f_3}{f_4} s_{44} s_{33} c_{22} c_{11} + \frac{f_3 f_1}{f_2 f_4} s_{44} s_{33} s_{22} s_{11}, \quad (C.39)$$

$$p(a) \eta_1'(a, \lambda) = -f_1 c_{44} c_{33} c_{22} s_{11} - f_2 c_{44} c_{33} s_{22} c_{11} - f_3 c_{44} s_{33} c_{22} c_{11}$$

$$-f_4 s_{44} c_{33} c_{22} c_{11} + \frac{f_3 f_1}{f_2} c_{44} s_{33} s_{22} s_{11} + \frac{f_1 f_4}{f_2} s_{44} c_{33} s_{22} s_{11}$$

$$+ \frac{f_1 f_4}{f_3} s_{44} s_{33} c_{22} s_{11} + \frac{f_2 f_4}{f_3} s_{44} s_{33} s_{22} c_{11}, \quad (C.40)$$

$$\eta_2(a, \lambda) = \frac{1}{f_1} c_{44} c_{33} c_{22} s_{11} + \frac{1}{f_2} c_{44} c_{33} s_{22} c_{11} + \frac{1}{f_3} c_{44} s_{33} c_{22} c_{11}$$

$$+ \frac{1}{f_4} s_{44} c_{33} c_{22} c_{11} - \frac{f_2}{f_1 f_3} c_{44} s_{33} s_{22} s_{11} - \frac{f_2}{f_1 f_4} s_{44} c_{33} s_{22} s_{11}$$

$$- \frac{f_3}{f_1 f_4} s_{44} s_{33} c_{22} s_{11} - \frac{f_3}{f_2 f_4} s_{44} s_{33} s_{22} c_{11}, \quad (C.41)$$

and

$$p(a) \eta_2'(a, \lambda) = c_{44} c_{33} c_{22} c_{11} - \frac{f_2}{f_1} c_{44} c_{33} s_{22} s_{11} - \frac{f_3}{f_1} c_{44} s_{33} c_{22} s_{11}$$

$$-\frac{f_3}{f_2} c_{44} s_{33} s_{22} c_{11} - \frac{f_4}{f_1} s_{44} c_{33} c_{22} s_{11} - \frac{f_4}{f_2} s_{44} c_{33} s_{22} c_{11}$$

$$- \frac{f_4}{f_3} s_{44} s_{33} c_{22} s_{11} + \frac{f_2 f_4}{f_1 f_3} s_{44} s_{33} s_{22} s_{11}. \quad (C.42)$$
Equation (C.23) gives that,

\[
D(\lambda) = 2c_{44}c_{33}c_{22}s_{11} - \left(\frac{f_1}{f_2} + \frac{f_2}{f_1}\right)c_{44}c_{33}s_{22}s_{11} - \left(\frac{f_1}{f_3} + \frac{f_3}{f_1}\right)c_{44}c_{33}s_{22}s_{11}
- \left(\frac{f_2}{f_3} + \frac{f_3}{f_2}\right)c_{44}s_{33}s_{22}s_{11} - \left(\frac{f_1}{f_4} + \frac{f_4}{f_1}\right)s_{44}c_{33}c_{22}s_{11} - \left(\frac{f_2}{f_4} + \frac{f_4}{f_2}\right)s_{44}c_{33}s_{22}s_{11} - \left(\frac{f_3}{f_4} + \frac{f_4}{f_3}\right)s_{44}s_{33}s_{22}s_{11} + \left(\frac{f_3 f_1}{f_2 f_4} + \frac{f_2 f_4}{f_1 f_3}\right)s_{44}s_{33}s_{22}s_{11}. \tag{C.43}
\]

In the region \(-2 \leq D(\lambda) \leq 2\), by Eq. (C.24) the band structure can be more explicitly written as

\[
\cos ka = \cos k_4 d_4 \cos k_3 d_3 \cos k_2 d_2 \cos k_1 d_1
- \frac{1}{2} \left(\frac{f_1}{f_2} + \frac{f_2}{f_1}\right) \cos k_4 d_4 \cos k_3 d_3 \sin k_2 d_2 \sin k_1 d_1
- \frac{1}{2} \left(\frac{f_1}{f_3} + \frac{f_3}{f_1}\right) \cos k_4 d_4 \sin k_3 d_3 \cos k_2 d_2 \sin k_1 d_1
- \frac{1}{2} \left(\frac{f_2}{f_3} + \frac{f_3}{f_2}\right) \cos k_4 d_4 \sin k_3 d_3 \sin k_2 d_2 \cos k_1 d_1
- \frac{1}{2} \left(\frac{f_1}{f_4} + \frac{f_4}{f_1}\right) \sin k_4 d_4 \cos k_3 d_3 \cos k_2 d_2 \sin k_1 d_1
- \frac{1}{2} \left(\frac{f_2}{f_4} + \frac{f_4}{f_2}\right) \sin k_4 d_4 \cos k_3 d_3 \sin k_2 d_2 \cos k_1 d_1
- \frac{1}{2} \left(\frac{f_3}{f_4} + \frac{f_4}{f_3}\right) \sin k_4 d_4 \sin k_3 d_3 \cos k_2 d_2 \cos k_1 d_1
+ \frac{1}{2} \left(\frac{f_3 f_1}{f_2 f_4} + \frac{f_2 f_4}{f_1 f_3}\right) \sin k_4 d_4 \sin k_3 d_3 \sin k_2 d_2 \sin k_1 d_1. \tag{C.44}
\]

For layered crystals of \(N = 5\) or more, similar equations can be straightforwardly obtained.

Relevant expressions for the dispersion relations were obtained in the literature, see, for example [6–9]. The approach used here is more basic and simpler and provides more useful results. \(\eta_i(a, \lambda)\) and \(p(a)\eta'_i(a, \lambda)\), \(i = 1, 2\), play a substantial role in investigations of the existence and properties of surface states/modes in one-dimensional semi-infinite layered crystals such as in Appendices A, E, and F.

Equations (C.19)–(C.24) could be easily used in numerical investigations on layered crystals.
References

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Appendix D

Analytical Expressions of $\frac{\partial \Lambda}{\partial \tau}$ and $\frac{\partial \Lambda}{\partial \sigma}$

One of the particularly interesting recent progress in the Sturm–Liouville theory [1] is that mathematicians have found that the eigenvalues of regular Sturm–Liouville problems are differentiable functions of boundary locations, boundary conditions, as well as coefficients in the differential equation. Furthermore, the expressions of their derivatives have been obtained [2–4]. This new progress might find interesting applications in physics.

In Chap. 3 we presented a general analysis on the existence and properties of surface states caused by the termination of the periodic potential in one-dimensional semi-infinite electronic crystals. As an application of the theory of periodic Sturm–Liouville equations, in this Appendix we extend the investigations therein to further obtain equations on how the eigenvalue of an existing surface state/mode in a one-dimensional semi-infinite crystal depends on the boundary location and boundary condition, by following an approach developed by Kong and Zettl [3, 4]. The results obtained here are valid for the properties of an existing surface state/mode in more general one-dimensional semi-infinite crystals, including electronic crystals, photonic crystals, and phononic crystals as well.4

We are interested in a periodic Sturm–Liouville equation (2.2):

$$[p(x)y'(x)]' + [\lambda w(x) - q(x)]y(x) = 0,$$

where $p(x) > 0$, $w(x) > 0$ and $p(x)$, $q(x)$ and $w(x)$ are piecewise continuous real periodic functions with a finite period $a$:

$$p(x + a) = p(x), \quad q(x + a) = q(x), \quad w(x + a) = w(x).$$

We assume that Eq. (D.1) is solved, and all solutions are known. The eigenvalues are permitted bands $\epsilon_n(k)$, and the corresponding eigenfunctions are Bloch functions

---

4Parts of the work presented in this Appendix and corresponding numerical confirmations were published in [5].
\( \phi_n(k, x) \), where \( n = 0, 1, 2, \ldots \), and \( -\frac{\pi}{a} < k \leq \frac{\pi}{a} \). We are mainly interested in cases where there is always a band gap between two consecutive permitted eigenvalue bands. The band gaps of Eq. (D.1) are always located either at the center of the Brillouin zone \( k = 0 \) or the boundary of the Brillouin zone \( k = \frac{\pi}{a} \).

For a one-dimensional semi-infinite crystal, we assume that the original periodicity remains inside the semi-infinite crystal. For such a one-dimensional semi-infinite crystal with a left boundary at \( \tau \), the eigenvalues \( \Lambda \), and eigenfunctions \( \psi(x) \) for a specific boundary condition at the boundary \( \tau \) are solutions of the differential equation

\[
[p(x)\psi'(x)]' + [\Lambda w(x) - q(x)]\psi(x) = 0, \quad \tau < x < \infty, \quad (D.2)
\]

with the boundary condition at \( \tau \):

\[
\sigma \psi(\tau) - p(\tau)\psi'(\tau) = 0, \quad (D.3)
\]

where \( \sigma \) is the ratio of the quasi-derivative \( p\psi' \) over the function \( \psi \) at the boundary location \( \tau \) that depends on the boundary condition. For example, for a surface state in an ideal electronic crystal, the boundary condition \( \psi(\tau) = 0 \) leads to that \( \sigma = \infty \); For a surface mode in a phononic crystal with a free boundary, the boundary condition \( p(\tau)\psi'(\tau) = 0 \) leads to that \( \sigma = 0 \). To have a localized surface state/mode within a band gap in the crystal, in most cases \( \sigma \) needs to be in \([0, \infty] \).

On the basis of that Eq. (D.1) is solved, the existence and the properties of the solutions of Eqs. (D.2) and (D.3) are completely determined by \( \tau \) and \( \sigma \) in Eq. (D.3).

In general, a solution of Eqs. (D.2) and (D.3) with an eigenvalue \( \Lambda \) within a band gap—if it exists—has a specific form. Its eigenfunction inside the semi-infinite one-dimensional crystal always has the form

\[
\psi(x, \Lambda) = e^{-\beta(\Lambda)x} f(x, \Lambda), \quad (D.4)
\]

where \( f(x, \Lambda) \) is a periodic function \( f(x + a, \Lambda) = f(x, \Lambda) \) if the band gap is at the center of the Brillouin zone \( k = 0 \), or a semi-periodic function \( f(x + a, \Lambda) = -f(x, \Lambda) \) if the band gap is at the boundary of the Brillouin zone \( k = \frac{\pi}{a} \). \( \beta(\Lambda) \) is a positive real number depending on \( \Lambda \). The exponential factor in Eq. (D.4) makes that \( \psi(x, \Lambda) \) is localized near the left end \( \tau \) of the semi-infinite crystal and thus is a surface state/mode. As \( \Lambda \) approaches a band edge, \( \beta \) decreases but remains to be finite as long as \( \Lambda \) does not reach the band edge. \( \psi(x, \Lambda) \) in Eq. (D.4) can always be chosen as a real function and,

\[
\psi(x, \Lambda) = 0, \quad x \to \infty, \quad (D.5)
\]

and can be normalized in the interval \((\tau, \infty)\):

\[
\int_\tau^\infty w(x)\psi^2(x, \Lambda)dx = 1. \quad (D.6)
\]
In the following, we try to investigate how the eigenvalue $\Lambda$ of an existing surface state/mode depends on $\tau$ and $\sigma$. We assume $\sigma \neq \infty$ at first. Let $\delta \sigma$ be an infinitesimal real number. Similar to that $\psi$ is a solution of Eqs. (D.2) and (D.3), we have a real solution $\chi$ of the following equation:

$$[p(x)\chi'(x)]' + [(\Lambda + \delta \Lambda)w(x) - q(x)]\chi(x) = 0, \quad \tau < x < \infty, \quad (D.7)$$

with the boundary condition

$$(\sigma + \delta \sigma)\chi(\tau) - p(\tau)\chi'(\tau) = 0. \quad (D.8)$$

$\chi$ will have properties similar to $\psi$ as described in Eqs. (D.4)–(D.6). From Eqs. (D.2) and (D.7) we obtain that

$$(p\psi')\chi - (p\chi')\psi = [\delta \Lambda]w\psi\chi, \quad \tau < x < \infty. \quad (D.9)$$

Since both $\psi$ and $\chi$ have the form of (D.4), we can do integrating with both sides of Eq. (D.9) in $(\tau, \infty)$ and obtain that

$$\int_\tau^{\infty} [(p\psi')\chi - (p\chi')\psi]dx = \int_\tau^{\infty} [\delta \Lambda]w\psi\chi dx \quad (D.10)$$

The left side of Eq. (D.10)

$$\int_\tau^{\infty} [(p\psi')\chi - (p\chi')\psi]dx = -[(p\psi')\chi - (p\chi')\psi]_{x=\tau}, \quad (D.11)$$

where Eq. (D.5) and thus $[(p\psi')\chi - (p\chi')\psi]_{x=\infty} = 0$ was used.

Let $\chi = \psi + \delta \psi$, and let $\delta \sigma \to 0$, the right side of Eq. (D.10) gives

$$\int_\tau^{\infty} [\delta \Lambda]w\psi\chi dx = \int_\tau^{\infty} [\delta \Lambda]w\psi\psi dx, \quad (D.12)$$

since $\int_\tau^{\infty} [\delta \Lambda]w\psi(\delta \psi)dx$ is a higher order infinitesimal number than $\int_\tau^{\infty} [\delta \Lambda]w\psi\psi dx$ as $\delta \sigma \to 0$ and thus is negligible.

Combining Eqs. (D.11) and (D.12), and using the normalization Eq. (D.6) of $\psi$ in Eq. (D.12), we obtain that

$$-[(p\psi')\chi - (p\chi')\psi]_{x=\tau} = \delta \Lambda. \quad (D.13)$$

For the case where $\sigma = \infty$, note that Eq. (D.3) now indicates $\psi(\tau) = 0$, the function $\chi$ can be chosen as the solution of

$$[p(x)\chi'(x)]' + [(\Lambda + \delta \Lambda)w(x) - q(x)]\chi(x) = 0, \quad \tau + \delta \tau < x < \infty, \quad (D.14)$$
under the boundary condition $\chi(\tau + \delta\tau) = 0$, where $\delta\tau$ is an infinitesimal real number. Let $\delta\tau \to 0$, very similar arguments lead to the same Eq. (D.13).

Several quantitative relationships between the eigenvalue $\Lambda$ and the boundary location $\tau$ or the boundary condition $\sigma$ can be obtained from Eq. (D.13).

1. The $\tau$-dependence of the eigenvalue with the boundary condition $\psi(\tau) = 0$.

Let the two eigenfunctions $\psi$ and $\chi$ satisfy $\psi(\tau) = 0$, and $\chi(\tau + \delta\tau) = 0$. Equation (D.13) leads to that

$$- p(\tau)\psi'(\tau)\chi(\tau) = \delta\Lambda. \quad \text{(D.14)}$$

$-\chi(\tau)$ on the left side of Eq. (D.14) is

$$-\chi(\tau) = \chi(\tau + \delta\tau) - \chi(\tau) = \int_\tau^{\tau + \delta\tau} \frac{1}{p(x)}[p(x)\chi'(x)]dx$$

$$= \int_\tau^{\tau + \delta\tau} \frac{1}{p(x)}[p(x)\psi'(x)]dx + \int_\tau^{\tau + \delta\tau} \frac{1}{p(x)}[p(x)\delta\psi'(x)]dx, \quad \text{(D.15)}$$

where $\chi(\tau + \delta\tau) = 0$, and $\chi = \psi + \delta\psi$ were used. By noting that as $\delta\tau \to 0$, the second term on the right side of Eq. (D.15) is a higher order infinitesimal quantity than the first term, and thus is negligible, we obtain that

$$p(\tau)\psi'(\tau) \left[ \frac{1}{p(\tau)} p(\tau)\psi'(\tau) \right] \delta\tau = \delta\Lambda.$$ 

That is, as $\delta\tau \to 0$,

$$\frac{\partial \Lambda}{\partial \tau} = \frac{1}{p(\tau)}[p(\tau)\psi'(\tau)]^2. \quad \text{(D.16)}$$

2. The $\tau$-dependence of the eigenvalue with the boundary condition $p(\tau)\psi'(\tau) = 0$.

Let the two eigenfunctions $\psi$ and $\chi$ satisfy $p(\tau)\psi'(\tau) = 0$ and $p(\tau + \delta\tau)\chi'(\tau + \delta\tau) = 0$. Then Eq. (D.13) leads to that

$$p(\tau)\chi'(\tau)\psi(\tau) = \delta\Lambda. \quad \text{(D.17)}$$

$p(\tau)\chi'(\tau)$ on the left side of Eq. (D.17) is

$$p(\tau)\chi'(\tau) = - \int_\tau^{\tau + \delta\tau} [p(x)\chi'(x)]'dx = - \int_\tau^{\tau + \delta\tau} [q(x) - (A + \delta A)w(x)]\chi(x)dx$$
Appendix D: Analytical Expressions of $\frac{\partial \Lambda}{\partial \tau}$ and $\frac{\partial \Lambda}{\partial \sigma}$

\[\quad = -\int_{\tau}^{\tau+\delta \tau} [q(x) - (\Lambda + \delta \Lambda)w(x)]\psi(x) dx - \int_{\tau}^{\tau+\delta \tau} [q(x) - (\Lambda + \delta \Lambda)w(x)]\delta \psi(x) dx, \quad (D.18)\]

where $p(\tau + \delta \tau)\chi'(\tau + \delta \tau) = 0$, Eq. (D.7), and $\chi = \psi + \delta \psi$ were used. By noting that in comparison with the first term on the right side of Eq. (D.18), the second term is a higher order infinitesimal quantity as $\delta \tau \to 0$ and thus is negligible, and $\delta \Lambda \to 0$, we obtain that

\[\psi(\tau)[-q(\tau)\psi(\tau) + \Lambda w(\tau)\psi(\tau)] \delta \tau = \delta \Lambda.\]

That is, as $\delta \tau \to 0$,

\[\frac{\partial \Lambda}{\partial \tau} = -[\psi(\tau)]^2[q(\tau) - \Lambda w(\tau)]. \quad (D.19)\]

3. The $\tau$-dependence of the eigenvalue with the boundary condition neither $p(\tau)\psi'(\tau)$ nor $\psi(\tau)$ is zero.

For the cases where the boundary condition is that neither $p(\tau)\psi'(\tau)$ nor $\psi(\tau)$ is zero, as pointed out in [3], we can combine the results of Eqs. (D.16) and (D.19) and obtain that

\[\frac{\partial \Lambda}{\partial \tau} = \frac{1}{p(\tau)}[p(\tau)\psi'(\tau)]^2 - [\psi(\tau)]^2[q(\tau) - \Lambda w(\tau)]. \quad (D.20)\]

4. The $\sigma$-dependence of the eigenvalue of the surface state with a specific boundary location $\tau$.

For the $\sigma$-dependence of the eigenvalue of the surface state near the neighborhood of $\sigma = 0$, note that $\sigma = 0$ means $p(\tau)\psi'(\tau) = 0$ then $\psi(\tau) \neq 0$, and thus $\chi(\tau) \neq 0$ for an infinitesimal $\delta \sigma$. By using Eqs. (D.3) and (D.8), Eq. (D.13) leads to that

\[\delta \sigma (\psi \chi)_{x=\tau} = \delta \Lambda.\]

Let $\delta \sigma \to 0$ we have $\chi \to \psi$ and obtain that

\[\frac{\partial \Lambda}{\partial \sigma} = [\psi(\tau)]^2. \quad (D.21)\]

For the $\sigma$-dependence of the eigenvalue of the surface state not near the neighborhood of $\sigma = 0$, then $p(\tau)\psi'(\tau) \neq 0$ and thus $p(\tau)\chi'(\tau) \neq 0$ for an infinitesimal $\delta \sigma$. By using Eqs. (D.3) and (D.8), Eq. (D.13) leads to that

\[p(\tau)\psi'(\tau)p(\tau)\chi'(\tau)\sigma^{-2}(\delta \sigma) = \delta \Lambda.\]
Let $\delta \sigma \to 0$ we have $\chi'(\tau) \to \psi'(\tau)$ and obtain that

$$\frac{\partial \Lambda}{\partial \sigma} = \sigma^{-2} [p(\tau)\psi'(\tau)]^2 = [\psi(\tau)]^2 > 0,$$

the same as in Eq. (D.21).

Equations (D.20) and (D.21) are two general equations indicating how the eigenvalue of an existing surface state/mode depends on $\tau$ and $\sigma$ quantitatively. The obtained equations were verified by numerical calculations [5].

Equations (D.20) and (D.21) can be considered as further generalizations and quantifications of two equations (3.7) and (3.8) in Chap. 3. In particular, for an existing surface state in a one-dimensional semi-infinite electronic crystal:

(i) Equation (D.21) is a quantitative equation of Eq. (3.7) in Chap. 3;

(ii) Equation (D.20) is a quantitative equation of Eq. (3.8) in Chap. 3. For such a case, Eq. (D.20) can be rewritten as

$$\frac{\partial \Lambda}{\partial \tau} = \left[ \frac{1}{p(\tau)} \sigma^2 + \Lambda - q(\tau) \right].$$

$\frac{\partial \Lambda}{\partial \tau} > 0$ if $\frac{1}{p(\tau)} \sigma^2 + \Lambda > q(\tau)$, which corresponds to that the “reduced outside potential” at the surface, is higher than the “reduced periodic potential” $q(\tau)$.

For a specific $\sigma$, $\Lambda(\tau)$ is surely a periodic function of $\tau$ with a period $a$, similar to coefficients $p, q, w$ in Eqs. (D.1) and (D.2). The result obtained here that $\frac{\partial \Lambda}{\partial \tau} > 0$ is true only when $\Lambda$ is the eigenvalue of an existing surface state/mode in the specific forbidden eigenvalue range at the boundary location $\tau$ with the specific $\sigma$. A direct consequence of $\frac{\partial \Lambda}{\partial \tau} > 0$ is that the termination of the periodicity at a boundary $\tau$ in a semi-infinite periodic system may or may not cause a surface state/mode in a specific forbidden eigenvalue range.

The results presented here may find practical applications in relevant problems, in particular, in investigating and designing periodic man-made systems such as photonic and phononic crystals.

References

Appendix E
One-Dimensional Phononic Crystals

Investigations on classical waves in periodically arranged alternative media, such as elastic waves in periodically alternating elastic mediums—often called phononic crystals—, electromagnetic waves in periodically alternating dielectric mediums—often called photonic crystals—, and so forth, have a long history in physics. See, for example, [1–4]. These problems received increasing attention in recent decades, due to their unusual physical properties observed in these heterostructures in comparison with bulk materials as well as the tremendous technical progress made in the fabrication of these man-made heterostructures [5–15]. The most interesting property of these heterostructures is the possible existence of forbidden frequency band gaps induced by the difference in the elastic or dielectric properties of the constituents and the periodicity of these systems, which can lead to valuable practical applications. One-dimensional phononic crystals or photonic crystals are the simplest phononic crystals or photonic crystals. A clear understanding of the one-dimensional problems provides a basis for further understandings of higher-dimensional systems.

The simplest cases are that such one-dimensional crystals are made of two different homogeneous and isotropic layered media alternatively. A primary theoretical formalism widely used for investigations of such layered structures is based on the Transfer Matrix Method (TMM). In this formalism one solves the corresponding wave equation in each layer, matches the solutions at the interfaces of adjacent layers according to the necessary continuous conditions, and then uses the Bloch theorem to treat the periodicity [6–8].

In comparison with the extensive literature on the investigations on classical waves in periodic media, the understanding of the effects of the very existence of the boundary or boundaries in such systems is relatively less. There are interesting investigations on semi-infinite layered phononic and photonic crystals in the literature, see, for example [5–9,11,16–28] and references therein. To the author’s knowledge, investigations focusing on the eigenmodes in one-dimensional phononic or photonic crystals of finite length $L = Na$—here $a$ is the period length of the crystal, and $N$ is a positive integer—began only recently [29–35].

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The author does not have much working experience and knows limitedly on the rich and colorful physics phenomena and their possible applications in these intensively investigated and still fast growing fields. Nevertheless, he feels that the problems studied in the major parts of this book—the effects of the boundary existence and the finite size on the electronic states in crystals—may have their correspondences in relevant problems of phononic crystals and photonic crystals. An advantage of the modern periodic Sturm–Liouville theory \cite{36–38} is that it can straightforwardly treat wave equations of many one-dimensional phononic crystals and photonic crystals. Based on the theory summarized in Chap. 2, a theoretical formalism to treat one-dimensional phononic crystals and photonic crystals—including the layered one-dimensional phononic crystals and photonic crystals—can be developed. This theoretical formalism treats a phononic crystal or photonic crystal as a whole from the beginning. Major relevant equations previously obtained based on TMM can be easily re-derived from the theory as specific cases. New equations for treating more general and complicated cases can be obtained, and more comprehensive understandings of relevant problems can also be achieved.

In this Appendix, we discuss one-dimensional phononic crystals, in the order of infinite size, semi-infinite size, and finite size. In Appendix F, we will investigate one-dimensional photonic crystals. We will focus on the general formalisms and general understandings, rather than the detailed distinctions between different specific materials. Since in many cases the wave equation for a one-dimensional phononic crystal or photonic crystal can be considered as a specific form of the periodic Sturm–Liouville equations (2.2), similarly as the Schrödinger equation for a one-dimensional electronic crystal, we will see that many fundamental understandings on the one-dimensional electronic crystals presented in Chaps. 3 and 4 do have their correspondences in one-dimensional phononic crystals and photonic crystals. Scientists working in these fields might find more interesting applications of the modern theory of periodic Sturm–Liouville theory in their specific problems.

E.1 One-Dimensional Phononic Crystals of Infinite Length

We begin by considering the propagation of transverse elastic waves in a simple one-dimensional phononic crystal as illustrated in Fig. E.1. The phononic crystal is assumed to be composed of two or more isotropic media, periodic in the \(x\) direction and homogeneous in the \(y\) and \(z\) directions \cite{30}.

By choosing the displacements to be in the \(y\) direction, the dynamic equation for the transverse acoustic waves is given by \cite{39}

\[
\rho(x) \frac{\partial^2 y(x, z, t)}{\partial t^2} = \frac{\partial}{\partial x} \left[ \mu(x) \frac{\partial y(x, z, t)}{\partial x} \right] + \mu(x) \frac{\partial^2 y(x, z, t)}{\partial z^2},
\]

where \(\rho(x + a) = \rho(x)\) is the density and \(\mu(x + a) = \mu(x)\) is the Lamé’s coefficient, they are periodic with period \(a\). By writing the displacements of the acoustic waves as
Fig. E.1  Schematic plot of a one-dimensional phononic crystal, in which the Lamé’s coefficient $\mu(x)$ and the density $\rho(x)$ are periodic functions of $x$. Reprinted with permission from S. Y. Ren and Y. C. Chang: Phys. Rev. B 75, 212301 (2007). Copyright by American Physical Society

\[
y(x, z, t) = y(x)e^{i(k_z z - \omega t)},
\]

the wave equation of the problem now has the form

\[
- [\mu(x)y'(x)]' + [\mu(x)k_z^2 - \rho(x)\lambda]y(x) = 0,
\]  

(E.1)

where $\lambda = \omega^2 \geq 0$, both $\mu(x) > 0$ and $\rho(x) > 0$. Equation (E.1) is a special case of the more general periodic Sturm–Liouville equations (2.2).

Most previous investigations on one-dimensional phononic crystals focused on their permitted band structure. By (2.54), the permitted band structure of a phononic crystal described by (E.1) is determined by its discriminant $D(\lambda)$ defined as

\[
D(\lambda) = \eta_1(a, \lambda) + \mu(a)\eta_2'(a, \lambda),
\]  

(E.2)

where $\eta_1(x, \lambda)$ and $\eta_2(x, \lambda)$ are two linearly independent normalized solutions of Eq. (E.1) satisfying

\[
\eta_1(0, \lambda) = 1, \quad \mu(0)\eta_1'(0, \lambda) = 0; \quad \eta_2(0, \lambda) = 0, \quad \mu(0)\eta_2'(0, \lambda) = 1.
\]  

(E.3)

In the $\lambda$ ranges where $-2 \leq D(\lambda) \leq 2$ the permitted eigenmode solutions $\phi_n(k_x, k_z, x)$ can exist as solutions of (E.1):

\[
\phi_n(k_x, k_z, x + a) = e^{ik_x a} \phi_n(k_x, k_z, x).
\]

The Bloch wave vector $k_x$ in the eigenfunction $\phi_n(k_x, k_z, x)$ and the eigenvalue $\varepsilon_n(k_x, k_z)$ is limited in the Brillouin zone,

\[
-\frac{\pi}{a} < k_x \leq \frac{\pi}{a}.
\]

\[5\]  
The mathematical theory in this section can also be applied to the cases where the longitudinal elastic waves propagate along the $x$ direction, which corresponds to $k_z = 0$. 

The permitted band structure of the phononic crystal can be obtained from $D(\lambda)$ in (E.2) as:

$$
cos k_x a = \frac{1}{2} D(\lambda),
$$

(E.4)

Many previously investigated one-dimensional phononic crystals are layered phononic crystals, see, for example, [1, 6, 16–24] and references therein. The simplest cases are that a one-dimensional layered phononic crystal is constructed of two different materials with Lamé’s coefficients $\mu_l$, densities $\rho_l$ and thicknesses $d_l$, where $l = 1, 2$. In such a case $\mu(x)$ and $\rho(x)$ in (E.1) can be written as

$$
\mu(x) = \begin{cases} 
\mu_1, & na < x \leq d_1 + na, \\
\mu_2, & na + d_1 < x \leq (n + 1)a,
\end{cases}
$$

(E.5)

and

$$
\rho(x) = \begin{cases} 
\rho_1, & na < x \leq d_1 + na, \\
\rho_2, & na + d_1 < x \leq (n + 1)a,
\end{cases}
$$

(E.6)

where $a = d_1 + d_2$ is the period, $n$ is an integer and $\mu_l > 0, \rho_l > 0$ are real constants. Now in Eq. (E.1) $\mu(x) = \mu_l$ and $\mu(x)k_z^2 - \rho(x)\lambda$ are piecewise continuous functions and discontinuous at isolated points $x = na$ and $x = d_1 + na$.

The Eq. (E.1) now can be written in the form

$$
[\mu_l y(x)]' + \mu_l k_z^2 y(x) = 0,
$$

(E.7)

by introducing

$$
\mu_l k_z^2 = \lambda \rho_l - \mu_l k_z^2,
$$

(E.8)

where $k_z$ is real if $\lambda \rho_l - \mu_l k_z^2 > 0$ or imaginary if $\lambda \rho_l - \mu_l k_z^2 < 0$.

From (C.31) in Appendix C, we obtain that

$$
D(\lambda) = 2 \cos k_2 d_2 \cos k_1 d_1 - \left( \frac{\mu_1 k_1}{\mu_2 k_2} + \frac{\mu_2 k_2}{\mu_1 k_1} \right) \sin k_2 d_2 \sin k_1 d_1.
$$

(E.9)

As $\lambda$ increases from $-\infty$, $D(\lambda)$ changes in the way similar to what was described in Sect. 2.4.

From (E.4) and (E.9) one obtains that for such a layered phononic crystal, the permitted band structure is determined by

$$
\cos k_x a = \cos k_2 d_2 \cos k_1 d_1 - \frac{1}{2} \left[ \frac{\mu_1 k_1}{\mu_2 k_2} + \frac{\mu_2 k_2}{\mu_1 k_1} \right] \sin k_2 d_2 \sin k_1 d_1,
$$

(E.10)
where $k_x$ is the Bloch wave vector. Equation (E.10) is essentially the dispersion relation frequently used in the literature, such as, in [1, 6, 10, 17, 18, 22, 24]. This approach can be easily extended to more general cases such as that each period unit contains more than two materials [20, 21] as shown in Appendix C.

For example, by (C.38), the dispersion relation of a one-dimensional layered phononic crystal composed of three different materials with Lamé’s coefficients $\mu_1, \mu_2, \mu_3$, densities $\rho_1, \rho_2, \rho_3$, and thicknesses $d_1, d_2, d_3$ can be written as

$$
\cos k_x a = \cos k_3 d_3 \cos k_2 d_2 \cos k_1 d_1 - \frac{1}{2} \left( \frac{\mu_1 k_1}{\mu_2 k_2} + \frac{\mu_2 k_2}{\mu_1 k_1} \right) \cos k_3 d_3 \sin k_2 d_2 \sin k_1 d_1 - \frac{1}{2} \left( \frac{\mu_1 k_1}{\mu_3 k_3} + \frac{\mu_3 k_3}{\mu_1 k_1} \right) \sin k_3 d_3 \cos k_2 d_2 \sin k_1 d_1 - \frac{1}{2} \left( \frac{\mu_2 k_2}{\mu_3 k_3} + \frac{\mu_3 k_3}{\mu_2 k_2} \right) \sin k_3 d_3 \sin k_2 d_2 \cos k_1 d_1, \quad (E.11)
$$

where $k_x$ is the Bloch wave vector, and $\mu_l k^2_l = \lambda_l \rho_l - \mu_l k^2_z, l = 1, 2, 3$.

### E.2 Surface Modes in Semi-infinite One-Dimensional Phononic Crystals

Surface modes in semi-infinite one-dimensional phononic crystals have been investigated theoretically and experimentally for many years, see, for example, [6, 16–19, 22–24] and references therein. Since the boundary location and boundary condition of a semi-infinite one-dimensional phononic crystal can be more flexibly designed and altered than that in an electronic crystal, the theoretical and experimental investigations on how the existence and properties of surface modes depend on these factors have an apparently practical significance.

In this section, we investigate this subject based on the theory of periodic Sturm–Liouville equations in Chap. 2. We assume that (E.1) is solved. The eigenvalues of (E.1), $\varepsilon_n(k_x, k_z)$ describe the phononic band structure, and the corresponding eigenfunctions are Bloch functions $\phi_n(k_x, k_z, x)$, where $n = 0, 1, 2, \ldots$ and $-\frac{\pi}{a} < k_x \leq \frac{\pi}{a}$. For brevity, the $k_z$ dependence of the eigenvalues and eigenfunctions will be kept implicit in the discussions below. We are mainly interested in cases where there is always a band gap between two consecutive bands of (E.1). For these cases, the band edges $\varepsilon_n(0)$ and $\varepsilon_n\left(\frac{\pi}{a}\right)$ occur in the order

$$
\varepsilon_0(0) < \varepsilon_0\left(\frac{\pi}{a}\right) < \varepsilon_1\left(\frac{\pi}{a}\right) < \varepsilon_1(0) < \varepsilon_2(0) < \varepsilon_2\left(\frac{\pi}{a}\right) < \varepsilon_3\left(\frac{\pi}{a}\right) < \varepsilon_3(0) < \varepsilon_4(0) < \cdots.
$$

The band gaps are between $\varepsilon_{2m}\left(\frac{\pi}{a}\right)$ and $\varepsilon_{2m+1}\left(\frac{\pi}{a}\right)$ or between $\varepsilon_{2m+1}(0)$ and $\varepsilon_{2m+2}(0)$, here $m = 0, 1, 2, \ldots$. 

For a semi-infinite phononic crystal with a left boundary at \( \tau \), the eigenmodes are solutions of

\[
- [\mu(x)\psi'(x, \Lambda)]' + [\mu(x)k_z^2 - \rho(x)\Lambda]\psi(x, \Lambda) = 0, \quad x \geq \tau, \quad (E.12)
\]

and a boundary condition at \( \tau \). The boundary condition at the surface \( \tau \), in general, can be written as

\[
\sigma \psi(\tau, \Lambda) - \mu(\tau)\psi'(\tau, \Lambda) = 0. \quad (E.13)
\]

We call a semi-infinite crystal given by (E.12) and (E.13) as a right semi-infinite crystal, for the convenience of later discussions.

For surface modes in one-dimensional semi-infinite phononic crystals, we are interested in the cases where \( \Lambda \) is in a frequency range \([\varepsilon_{2m}^{\frac{\pi}{a}}, \varepsilon_{2m+1}^{\frac{\pi}{a}}]\) or \([\varepsilon_{2m+1}(0), \varepsilon_{2m+2}(0)]\) or \( \Lambda \leq \varepsilon_0(0) \) of Eq. (E.1).\(^6\) By the theory in Sect. 2.5, for any \( \Lambda \) in such a range, two linearly independent solutions of Eq. (E.1) can always be chosen in such a way that one is non-divergent, and the other one is divergent in \([\tau, +\infty)\). Only when the one non-divergent solution of (E.1) also satisfies (E.13) can we have a solution of both (E.12) and (E.13). Such a solution of (E.12) in a range of \(|D(\Lambda)| \geq 2\) has the form

\[
\psi(x, \Lambda) = e^{-\beta(\Lambda)x} f(x, \Lambda), \quad (E.14)
\]

where \( \beta \geq 0 \), \( f(x, \Lambda) \) is a periodic function if \( \Lambda \) is in \([\varepsilon_{2m+1}(0), \varepsilon_{2m+2}(0)]\) or \( \Lambda \leq \varepsilon_0(0) \), or a semi-periodic function if \( \Lambda \) is in \([\varepsilon_{2m}(\frac{\pi}{a}), \varepsilon_{2m+1}(\frac{\pi}{a})]\).

Inside the semi-infinite crystal any solution \( \psi(x, \Lambda) \) of Eq. (E.12) can be expressed as a linear combination of two normalized solutions \( \eta_1 \) and \( \eta_2 \) of Eq. (E.1):

\[
\psi(x, \Lambda) = c_1 \eta_1(x, \Lambda) + c_2 \eta_2(x, \Lambda), \quad x \geq \tau, \quad (E.15)
\]

where \( \eta_1(x, \Lambda) \) and \( \eta_2(x, \Lambda) \) are two normalized solutions of Eq. (E.1) satisfying that

\[
\eta_1(\tau, \Lambda) = 1, \quad \mu(\tau)\eta_1'(\tau, \Lambda) = 0; \quad \eta_2(\tau, \Lambda) = 0, \quad \mu(\tau)\eta_2'(\tau, \Lambda) = 1. \quad (E.16)
\]

### E.2.1 Simple Cases

The simplest cases are that a one-dimensional semi-infinite phononic crystal has a stress-free boundary surface. It leads to the boundary condition at \( \tau \) as

\[
\mu(\tau)\psi'(\tau, \Lambda) = 0. \quad (E.17)
\]

\(^6\)For any \( \lambda \) inside a permitted band where \(-2 < D(\lambda) < 2\), there are two non-divergent solutions of Eq. (E.1), a linear combination of two such non-divergent solutions can always satisfy Eqs. (E.12) and (E.13).
Equation (E.17) corresponds to the case $\sigma = 0$ in Eq. (E.13). Equation (E.15) becomes

$$\psi(x, \Lambda) = c_1 \eta_1(x, \Lambda), \quad x \geq \tau,$$

(E.18)

by Eq. (E.16). Equations (E.14), (E.17), and (E.18) lead to that

$$\mu(\tau + a) \eta'_1(\tau + a, \Lambda) = 0$$

(E.19)

is a necessary condition for the existence of a surface mode in a range $|D(\lambda)| \geq 2$ under the boundary condition (E.17).

The simplest one-dimensional phononic crystals are composed of two different isotropic homogeneous media alternatively. Without losing generality, we need only consider the cases where the boundary $\tau$ is in the first medium, i.e. $0 \leq \tau \leq d_1$. For such a case, we can treat the one-dimensional phononic crystal made of two media as a special case of that made of three media with physical parameters $\mu_1, \mu_2, \mu_1$ and $\rho_1, \rho_2, \rho_1$ and thicknesses $d_1 - \tau, d_2, \tau$. From (C.34), Eq. (E.19) becomes

$$-\mu_1 k_1 \cos k_2 d_2 \sin k_1 d_1 - \mu_2 k_2 \sin k_2 d_2 \cos k_1 d_1$$

$$-\mu_2 k_2 \left(1 - \frac{\mu_1^2 k_1^2}{\mu_2^2 k_2^2}\right) \sin k_2 d_2 \sin k_1 (d_1 - \tau) \sin k_1 \tau = 0.$$  

(E.20)

It can be written as

$$\cos k_2 d_2 \sin k_1 d_1 + \frac{1}{2} \left(\frac{\mu_2 k_2}{\mu_1 k_1} + \frac{\mu_1 k_1}{\mu_2 k_2}\right) \sin k_2 d_2 \cos k_1 d_1$$

$$+ \frac{1}{2} \left(\frac{\mu_2 k_2}{\mu_1 k_1} - \frac{\mu_1 k_1}{\mu_2 k_2}\right) \sin k_2 d_2 \cos k_1 (d_1 - 2\tau) = 0,$$

where $k_1, k_2$ are given in (E.8).

By Theorem 2.8, in each forbidden range starting from $[0, \epsilon_0(0)]$, there is always one and only one solution $\Lambda = \nu_{\tau,n}$ of (E.19) for any specific boundary location $\tau$. For a one-dimensional phononic crystal composed of two different isotropic homogeneous media alternatively, it is a solution of Eq. (E.20). The ratio $P = \frac{\psi(\tau + a, \Lambda)}{\psi(\tau, \Lambda)}$ for such a solution is,

$$P = \eta_1(\tau + a, \Lambda)$$

(E.21)

by Eqs. (E.16) and (E.18).

Using $\Lambda = \nu_{\tau,n}$ obtained from (E.20) into (C.33), we obtain the value of the surface mode at $x = \tau + a$:
\[
\eta_1(\tau + a, \nu_{\tau,n}) = \cos k_2 d_2 \cos k_1 d_1 - \frac{1}{2} \left[ \frac{\mu_1 k_1}{\mu_2 k_2} + \frac{\mu_2 k_2}{\mu_1 k_1} \right] \sin k_2 d_2 \sin k_1 d_1 \\
- \frac{1}{2} \left[ \frac{\mu_1 k_1}{\mu_2 k_2} - \frac{\mu_2 k_2}{\mu_1 k_1} \right] \sin k_2 d_2 \sin k_1 (d_1 - 2\tau). \tag{E.22}
\]

There are three possibilities for the obtained \( P = \eta_1(\tau + a, \Lambda) \) from (E.22): (a) \( 0 < |\eta_1(\tau + a, \nu_{\tau,n})| < 1 \); (b) \( |\eta_1(\tau + a, \nu_{\tau,n})| = 1 \); and (c) \( |\eta_1(\tau + a, \nu_{\tau,n})| > 1 \). The case (a) corresponds to an oscillatory decreasing solution \( \psi(x, \nu_{\tau,n}) = c_1 \eta_1(x, \nu_{\tau,n}) \) of Eqs. (E.12) and (E.17), a localized surface mode having the form of (E.14) with \( \beta(\nu_{\tau,n}) > 0 \). From Eqs. (E.20) and (E.22), one can easily obtain the expressions previously used such as in [6].

Similarly, for cases where a one-dimensional phononic crystal is composed of three different isotropic homogeneous media alternatively, we need only consider the cases where the boundary \( \tau \) is in the first medium, i.e. \( 0 \leq \tau \leq d_1 \). We can treat the one-dimensional phononic crystal made of three media considered here as a special case of a one-dimensional phononic crystal made of four media with physical parameters \( \mu_1, \mu_2, \mu_3, \mu_1 \) and \( \rho_1, \rho_2, \rho_3, \rho_1 \) and thicknesses \( d_1 - \tau, d_2, d_3, \tau \). For such a case, equations corresponding to Eqs. (E.20) and (E.22) can be obtained from (C.39)–(C.42).

### E.2.2 More General Cases

For more general cases \( \sigma \neq 0 \), Eqs. (E.13) and (E.14) lead to that

\[
\sigma \psi(\tau + a, \Lambda) - \mu(\tau) \psi'(\tau + a, \Lambda) = \sigma \psi(\tau, \Lambda) - \mu(\tau) \psi'(\tau, \Lambda) = 0 \tag{E.23}
\]

is a necessary condition for the existence of a localized surface mode with a more general boundary condition (E.13).

From Eqs. (E.23), (E.15) and (E.14), reasonings similar to Sect. 3.5 lead to that the existence and properties of a surface mode in the one-dimensional semi-infinite phononic crystal are determined by the following two equations. They are

\[
\sigma = \frac{-\eta_1(\tau + a, \Lambda) + \mu(\tau) \eta_2'(\tau + a, \Lambda) - \sqrt{D^2(\Lambda) - 4}}{2 \eta_2(\tau + a, \Lambda)}, \tag{E.24}
\]

---

\(^7\) The case (b) corresponds to that Eq. (E.19) or Eq. (E.20) gives a band-edge eigenvalue of Eq. (E.7), \( \nu_{\tau,n} = \epsilon_\ell(k_g, k_z) \). Thus, \( \psi(x, \nu_{\tau,n}) \) is either a periodic function or a semi-periodic function in the semi-infinite phononic crystal. The case (c) corresponds to an oscillatory increasing solution \( \psi(x, \nu_{\tau,n}) \) of Eq. (E.19). A surface mode can exist in the complementary left semi-infinite phononic crystal in \( (-\infty, \tau] \).
for a band gap at the center of Brillouin zone $k_x = 0$, and

$$
\sigma = \frac{-\eta_1(\tau + a, \Lambda) + \mu(\tau)\eta'_2(\tau + a, \Lambda) + \sqrt{D^2(\Lambda) - 4}}{2 \eta_2(\tau + a, \Lambda)},
$$

(E.25)

for a band gap at the boundary of Brillouin zone $k_x = \frac{\pi}{a}$. Here $D(\lambda) = \eta_1(\tau + a, \lambda) + \mu(\tau)\eta'_2(\tau + a, \lambda)$ is the discriminant of Eq. (E.1).

Equations (E.24) and (E.25) are two equations which can be used to generally investigate the existence and properties of surface modes in a semi-infinite one-dimensional phononic crystal.

Similar to Sect. E.2.1, the simplest one-dimensional phononic crystals are those composed of two different media with Lamé’s coefficients $\mu_l$, densities $\rho_l$ and thicknesses $d_l$, where $j = 1, 2$. Without losing generality, we need only consider the cases where the boundary $\tau$ is in the first medium, i.e. $0 \leq \tau \leq d_1$. We can treat the one-dimensional phononic crystal as a special case of that made of three media with physical parameters $\mu_1, \mu_2, \mu_1; \rho_1, \rho_2, \rho_1$; and thicknesses $d_1 - \tau, d_2, \tau$. The existence and properties of surface modes in such a one-dimensional semi-infinite crystal can be investigated by using Eqs. (E.24) and (E.25) with $\eta_i, \mu \eta'_i, i = 1, 2$ given in (C.33)–(C.36).

Similarly, the existence and properties of surface modes in a layered semi-infinite crystal composed of three homogeneous isotropic media can be investigated by using Eqs. (E.24) and (E.25) with $\eta_i, \mu \eta'_i, i = 1, 2$ given in (C.39)–(C.42), etc.

If needed, surface modes in a one-dimensional phononic crystal composed of four or more different isotropic homogeneous media alternatively can be investigated similarly.

### E.2.3 Brief Discussions

A one-dimensional semi-infinite phononic crystal may or may not have a surface mode in a specific forbidden range: (E.24) or (E.25) may or may not have a solution in such a range. Equation (E.23) is a necessary but not sufficient condition for having a surface mode in a specific forbidden range.

If there is a solution $\Lambda$ of Eq. (E.23) existing in a specific forbidden range where $|D(\lambda)| \geq 2$, then $\Lambda$ can be either at a band edge or inside the forbidden range. Only when $\Lambda$ is inside the forbidden range, and the solution of (E.23) has the form of (E.14), we can have a surface mode solution of (E.12) and (E.13) in the right semi-infinite phononic crystal.

If $\Lambda$ is at a band edge, then the solution $\psi(x, \Lambda)$ of (E.23) will be a band-edge mode that is a periodic function or a semi-periodic function, depending on whether the band gap is at the center or the boundary of the Brillouin zone.
In the cases where $\sigma = 0$ in (E.23), if there is a surface mode $\Lambda = \nu_{\tau,n}$, the frequency of such a surface mode is below the corresponding permitted band, by Theorem 2.8.

Based on Theorem 2.8 in Chap. 2 on the zeros of solutions of (E.7), we can understand that the surface mode below the lowest bulk band has no zero in $(-\infty, +\infty)$, the surface mode in the lowest band-gap has one zero in $[0, a)$, and the surface mode in the second lowest band-gap has two zeros in $[0, a)$, ..., etc. Theorem 2.8 gives explanations on the behaviors of surface modes shown in several previous investigations. For example, the surface mode in Fig. 9a of Ref. [6] corresponds to a mode below $\varepsilon_{0}(0)$ thus has no zero; and the surface modes in Fig. 9b corresponds to a mode in the second lowest band-gap thus has two zeros in each unit cell. The theorem also explains the modes in Fig. 4 of Ref. [20], where each sub-figure corresponds to the surface mode in the following ranges: (a) below $\varepsilon_{0}(0)$; (b) in $(\varepsilon_{1}(0), \varepsilon_{2}(0))$; (c) in $(\varepsilon_{0}(\pi/a), \varepsilon_{1}(\pi/a))$; and (d) in $(\varepsilon_{2}(\pi/a), \varepsilon_{3}(\pi/a))$ respectively. Thus, each has no zero, two zeros, one zero and three zeros in a unit cell.

In this section, we have only treated surface modes in a semi-infinite crystal (without a cap layer) for simplicity. A slightly extended formalism can be developed to treat surface modes in a semi-infinite crystal with a cap layer, where the left sides in Eqs. (E.24) and (E.25) will be mathematical expressions containing parameters of the cap layer such as thickness, density, Lamé’s coefficient, and so forth.

### E.3 One-Dimensional Phononic Crystals of Finite Length

The mathematical theory in Chap. 2 can also be applied to treat the eigenmodes in a one-dimensional phononic crystal described by (E.1) with a finite length $L = Na$. Exact and general fundamental understandings of the eigenmodes in a one-dimensional phononic crystal of finite length with free surfaces can be analytically obtained.\(^8\)

For a one-dimensional phononic crystal described by (E.1) with two free surfaces at $x = \tau$ and $x = \tau + L$, where $L = Na$ and $N$ is an integer, the eigenvalues $\Lambda$ and the eigenfunctions $\psi(x)$ in the finite crystal are solutions of the differential equation

$$- [\mu(x)\psi'(x, \Lambda)]' + [\mu(x)k_z^2 - \rho(x)\Lambda]\psi(x, \Lambda) = 0, \quad \tau < x < \tau + L,$$

(E.26)

with the stress-free boundary condition at $x = \tau$ and $x = \tau + L$:

$$\mu(\tau)\psi'(\tau, \Lambda) = \mu(\tau)\psi'(\tau + L, \Lambda) = 0.$$

(E.27)

---

\(^8\)Part of the results in this subsection was published in [30]. Since the author did not know then that the theory of the Hill’s equation in [40] could be extended as presented in Chap. 2, $\mu'(x)$ rather than $\mu(x)$ was more restrictively assumed to be piecewise continuous.
Suppose $y_1(x, \lambda)$ and $y_2(x, \lambda)$ are two linearly independent solutions of (E.1). In general, a nontrivial solution of (E.26) and (E.27), if it exists, can be expressed as

$$\psi(x, \Lambda) = c_1 y_1(x, \Lambda) + c_2 y_2(x, \Lambda), \quad \tau < x < \tau + L,$$

(E.28)

—in which $c_1$ and $c_2$ are not both zero—and is a nontrivial solution of (E.1) satisfying (E.27).

The forms of two linearly independent solutions $y_1(x, \lambda)$ and $y_2(x, \lambda)$ in (E.28) can be determined by the discriminant $D(\lambda)$ of (E.1). The existence and the properties of nontrivial solutions of Eqs. (E.26) and (E.27) can be obtained on this basis.

For a one-dimensional phononic crystal of finite length, both the permitted bands and the forbidden $\lambda$ ranges of the infinite crystal should be considered. We need to consider the solutions of Eq. (E.27) for $\lambda$ in $[0, +\infty)$. According to the theory in Sect. 2.5, there are five different cases for the linearly independent solutions $y_1(x, \lambda)$ and $y_2(x, \lambda)$ depending on $D(\lambda)$. For the problem we are interested in here, they can be classified into two different $\lambda$ ranges: $\lambda$ is inside a permitted band, or not inside a permitted band.

### E.3.1 $\lambda$ Is inside a Permitted Band

In this case, $\lambda$ is inside a permitted band of (E.1), $-2 < D(\lambda) < 2$. By (2.73), two linearly independent solutions of (E.1) can be chosen as:

$$y_1(x, \lambda) = e^{i k_x(\lambda)x} p_1(x, \lambda),$$

$$y_2(x, \lambda) = e^{-i k_x(\lambda)x} p_2(x, \lambda).$$

(E.29)

Correspondingly we have

$$\mu(x + a) y_1'(x + a, \lambda) = e^{i k_x(\lambda)a} \mu(x) y_1'(x, \lambda),$$

$$\mu(x + a) y_2'(x + a, \lambda) = e^{-i k_x(\lambda)a} \mu(x) y_2'(x, \lambda),$$

(E.30)

where $k_x(\lambda)$ is a real number depending on $\lambda$ and

$$0 < k_x(\lambda)a < \pi.$$

From (E.27) and using (E.30) for $N$ times, we obtain that

$$c_1 \mu(\tau) y_1'(\tau, \Lambda) + c_2 \mu(\tau) y_2'(\tau, \Lambda) = 0,$$

$$c_1 e^{i k_x(\Lambda)L} \mu(\tau) y_1'(\tau, \Lambda) + c_2 e^{-i k_x(\Lambda)L} \mu(\tau) y_2'(\tau, \Lambda) = 0.$$
The zeros of $\mu(x)y_1'(x, \lambda)$ are separated from the zeros of $\mu(x)y_2'(x, \lambda)$. Thus, the existence of nontrivial solutions of (E.26) and (E.27) requires that

$$e^{ik_x(\Lambda)L} - e^{-ik_x(\Lambda)L} = 0.$$  

(E.31)

Note (E.31) does not contain $\tau$. The nontrivial solutions of the form (E.28) with (E.29) can exist if

$$k_x(\Lambda)L = j\pi,$$

where $j$ is a positive integer. There are $N - 1$ Bloch wave vector $k_x$ satisfying

$$k_x(\Lambda_{n,j}) = \frac{j\pi}{L}, \quad j = 1, 2, \ldots, N - 1.$$

Correspondingly, for each permitted band, there are $N - 1$ solutions of (E.26) and (E.27) whose eigenvalues are given by

$$\Lambda_{n,j} = \varepsilon_n\left(\frac{j\pi}{L}\right), \quad j = 1, 2, \ldots, N - 1.$$  

(E.32)

Each eigenvalue for this case is a function of $L$, the crystal length. However, all do not depend on the location of the crystal boundary $\tau$ or $\tau + L$. These modes $\psi(x, \Lambda_{n,j})$ are stationary Bloch modes consisting of two Bloch waves with wave vectors $k_x = \frac{j\pi}{L}$ and $-k_x = -\frac{j\pi}{L}$ in the finite crystal. For simplicity, we call these modes as $L$-dependent modes, although only the eigenvalue of such a mode depends only on $L$. The energies $\Lambda_{n,j}$ in (E.32) coincide with the band structure $\varepsilon_n(k_x)$ of the unconfined phononic crystal exactly. This case is very similar to the $L$-dependent confined electronic states discussed in Chap. 4. A noteworthy point is that although the boundary condition (E.27) is different from the boundary condition (4.6), the expressions of eigenvalues of the $L$-dependent states or modes for these two cases are the same.

### E.3.2 $\lambda$ is not Inside a Permitted Band

If $\lambda$ is not inside a permitted band, it may be inside a band gap or at a band edge.

\footnote{Otherwise, we have

$$c_1 \mu(\tau)y_1'(\tau, \Lambda) = 0, \quad \text{and} \quad c_2 \mu(\tau)y_2'(\tau, \Lambda) = 0.$$}

Since $\mu(\tau)y_1'(\tau + a, \Lambda) = e^{\pm k_x a}\mu(\tau)y_1'(\tau, \Lambda)$, we must have $\mu(\tau)y_1'(\tau + a, \Lambda) = 0$ if we have $\mu(\tau)y_1'(\tau, \Lambda) = 0$. By Theorem 2.8, this can happen only in the intervals where $|D(\Lambda)| \geq 2$. Thus, neither $\mu(\tau)y_1'(\tau, \Lambda)$ nor $\mu(\tau)y_2'(\tau, \Lambda)$ here can be zero. Therefore, this case leads to $c_1 = c_2 = 0$ and that no nontrivial solution of (E.26) and (E.27) exists from such a case.
If \( \lambda \) is inside a band gap, \( y_1(x, \lambda) \) and \( y_2(x, \lambda) \) can be chosen as in (2.77) if the band gap is at \( k_x = 0 \) \((D(\lambda) > 2)\) or as in (2.81) if the band gap is at \( k_x = \pi/a \) \((D(\lambda) < -2)\). By using a similar approach as we used to obtain (E.31), we obtain that

\[
\mu(\tau)\psi'(\tau + a, \Lambda) = \mu(\tau)\psi'(\tau, \Lambda) = 0 \tag{E.33}
\]

is a necessary condition for the existence of a solution of (E.26) and (E.27) for \( \lambda \) inside a band gap, since \( e^{\beta(\Lambda)L} - e^{-\beta(\Lambda)L} \neq 0 \) with a real \( \beta(\Lambda) \) \(\neq 0\).

If \( \lambda \) is at a band edge of Eq. (E.1), \( y_1(\lambda, x) \) and \( y_2(\lambda, x) \) can be chosen as in (2.75) if the band edge is at \( k_x = 0 \) \((D(\lambda) = 2)\) or as in (2.79) if the band gap is at \( k_x = \pi/a \) \((D(\lambda) = -2)\). Simple mathematics also gives that (E.33) is a necessary condition for the existence of a solution of (E.26) and (E.27).

Therefore, an existing solution of Eqs. (E.26) and (E.27) with its \( \Lambda \) not inside a permitted band must have the form of \( \psi(x, \Lambda) = e^{\pm\beta(\Lambda)}f(x, \Lambda) \) where \( \beta(\Lambda) \geq 0 \) and \( f(x, \Lambda) \) is a periodic function or a semi-periodic function. (E.33) is also a sufficient condition for the existence of a solution of (E.26) and (E.27) since from (E.33) we have that

\[
\mu(\tau)\psi'(\tau + \ell a, \Lambda) = \mu(\tau)\psi'(\tau, \Lambda) = 0, \tag{E.34}
\]

where \( \ell = 1, 2, \ldots, N \). Therefore (E.33) is a necessary and sufficient condition for the existence of a solution of (E.26) with the boundary condition (E.27) where \( \Lambda \) is not inside a permitted band.

Such eigenvalues can be written as \( \Lambda_{\tau,n} \), \( n = 0, 1, 2, \ldots \). The eigenvalues \( \Lambda_{\tau,n} \) obtained from (E.33) is the \( \nu_{\tau,n} \) given in (2.95). Equation (E.33) does not contain the crystal length \( L \); thus, an eigenvalue \( \Lambda_{\tau,n} \) of (E.26) and (E.27) obtained from (E.33) is only dependent on \( \tau \), but not on \( L \). For simplicity, we call the corresponding eigenmodes as the \( \tau \)-dependent modes.

Theorem 2.8 indicates that for any real number \( \tau \), there is always one and only one eigenvalue \( \nu_{\tau,n} \) below or equal to the minimum of the corresponding permitted band, determined by (E.33). Such as, \( \nu_{\tau,0} \) is in the interval \([0, \varepsilon_0(0)]\), \( \nu_{\tau,2m+1} \) is in the interval \([\varepsilon_{2m}(\frac{a}{L}), \varepsilon_{2m+1}(\frac{a}{L})]\), \( \nu_{\tau,2m+2} \) is in the interval \([\varepsilon_{2m+1}(0), \varepsilon_{2m+2}(0)]\), etc. Since in one-dimensional phononic crystals, each permitted band and each forbidden range exist alternatively, we can say that there is always one and only one \( \tau \)-dependent mode corresponding to each permitted band in a finite phononic crystal of length \( L = Na \). This case is similar to the \( \tau \)-dependent electronic states discussed in Chap. 4.

As discussed in Sect. E.2.2, the calculated \( P = \frac{\psi(\tau + a, \Lambda)}{\psi(\tau, \Lambda)} \) from (E.33) can have three possibilities: (a) \( 0 < |P| < 1 \); (b) \( |P| = 1 \); (c) \( |P| > 1 \). The case (a) corresponds to an oscillatory decreasing solution in the \( +x \) direction \( \psi(x, \Lambda) \) of Eqs. (E.26) and (E.27), a surface mode localized at the left boundary \( \tau \); The case (b) corresponds to that \( \psi(x, \Lambda) \) in Eq. (E.33) is a band-edge mode of Eq. (E.1); The case (c) corresponds to an oscillatory increasing solution \( \psi(x, \Lambda) \) in the \( +x \) direction, indicating a surface mode localized at the right boundary \( \tau + L \).

A significant difference is that the \( \tau \)-dependent mode here always has a lower frequency than the \( L \)-dependent modes corresponding to the same permitted band.
That is, the confinement in a one-dimensional phononic crystal of finite length due to
the boundary condition (E.27) always makes the $\tau$-dependent states go lower, rather
than always making the $\tau$-dependent states go higher in the quantum confinement
of electronic states as discussed in Chap. 4. The basic reason for this significant
difference is the difference between (E.27) and the boundary conditions (4.6) for
electronic states. As we see in Chap. 4, the boundary conditions (4.6) leads to the
requirement $y(\tau) = y(\tau + a) = 0$ for a forbidden range. Theorem 2.8 requires that
the corresponding eigenvalues must be in the band gap above the energy band. It is
this difference that makes the $\tau$-dependent states in finite one-dimensional phononic
crystals different from those in Chap. 4.

In conclusion, there are two different types of confined modes in a one-dimensional
phononic crystal of finite length $L = Na$. Of them, one type is that $N - 1$ modes
in each permitted band whose eigenvalue depends on the crystal size $L$ but not on
the crystal boundary $\tau$. The other type is one and only one confined mode in each
forbidden range below the permitted band, whose eigenvalue depends on the crystal
boundary $\tau$ but not the crystal length $L$.

Above results were obtained from a theory of differential equations approach,
which is most suitable to treat solid-solid phononic crystals. One-dimensional finite
phononic crystals of other forms were investigated in [29, 31, 33–35]. Similar results
were obtained. There are two types of confined phonon modes in a finite one-
dimensional phononic crystal containing $N$ cells: Corresponding to each permitted
band, there are $N - 1$ modes in the band whose frequencies depend on crystal size $N$;
whereas there is always one and only one mode in each forbidden range whose
frequency depends on the boundary location.

A.-C. Hladky, G. Allan and M. de Billy [29] investigated theoretically and exper-
imentally the propagation of longitudinal elastic waves along a one-dimensional
diatomic chain made of steel spheres of two different diameters alternatively. The
vibration modes of the infinite chain have two low-frequency branches, separated by
a band gap. In cases of a finite chain of $N$ unit periods, they obtained two different
types of modes: $N - 1$ vibration modes in each permitted band whose frequencies
strongly depend on $N$ and two modes whose frequency does not depend on $N$: one
in the band gap and the other always at a zero frequency.

By using a Green’s function method, El Hassouani et al. [31, 33] and El Boudouti
et al. [34] did theoretical investigations on acoustic modes in finite one-dimensional
structures made of $N$-periods, where each period is alternatively composed of a solid
(such as Plexiglas) layer and a fluid (such as water) layer, and the finite phononic
crystal is free of stress on both sides. They obtained two types of modes: $N - 1$ modes
whose frequencies depend on $N$ but not the boundary location in each permitted band,
and, one mode with a frequency depending on the boundary location but not $N$ in
each forbidden range. This latter is either a surface mode or a confined band-edge
mode.

El Boudouti and Djafari-Rouhani [35] further investigated the modes in semi-
infinite and finite one-dimensional phononic crystals constructed of more general
discrete or continuous media by using a Green’s function approach and obtained
similar results. They obtained a general expression for the Green’s function of a
finite crystal containing $N$ unit cells. The unit cell can be a multilayer structure or a multi-waveguide system, etc. The expression involves the relevant matrix elements of the Green’s function of the unit cell, but not the details of the unit cell. Thus, a general understanding of the eigenmodes of a finite crystal containing $N$ unit cell can be obtained without knowing the details of the unit cell. From such an expression for a finite crystal of $N$ unit cells, they obtained $N - 1$ confined modes in each bulk permitted band and an additional mode for each forbidden range. This additional mode is either a surface mode localized near one of the two ends if the unit cell is not symmetrical or a confined band edge mode if the unit cell is symmetrical. These extra modes are independent of $N$ and determined by the Green’s function of the unit cell.

In summary, in all different one-dimensional phononic crystals of finite size with $N$ unit cells that have been investigated so far, the eigen modes have common general properties if the modes are completely confined to the finite size of the crystal. There are two different types of eigen modes: In each permitted band there are $N - 1$ modes whose eigenvalues depend on the crystal size $N$ but not the boundary location $\tau$, and the eigenvalues of those modes can be obtained from the bulk dispersion relation; There is always one and only one mode corresponding to each forbidden range whose eigenvalue depends on the boundary location $\tau$ but not the crystal size $N$, and this mode is either a surface mode or a confined band-edge mode.

References

Appendix F
One-Dimensional Photonic Crystals

The interests in one-dimensional photonic crystals in the form of periodic multi-layer dielectric stacks have a long history. As early as hundreds of years ago, Hooke and Newton proposed the optical properties of stacks of thin layers [1, 2]. More recent investigations before late 1980’s can be found in [3–9] and references therein. The publication of two papers [10, 11] in 1987 indicated a significant breakthrough in investigations of photonic crystals and stimulated a rapid growth of research papers in this active and fruitful field in recent years [12–24]. Nowadays, much research attentions in optics is directed at exploring effects of periodicity in photonic micro- and nanostructures [25].

The most interesting property of the photonic crystals is the possible existence of forbidden frequency band gaps originated from the difference in the electromagnetic properties of the construction media and the periodicity of the systems, which has a high potential to lead to many interesting and valuable practical applications. The Maxwell equations on photonic crystals involve two different but closely related vector fields—the electric field $E$ and the magnetic field $H$—thus, the relevant physics is more plentiful and colorful in comparison with that of phononic crystals. The construction materials of photonic crystals can be more diversified; even where the medium outside a photonic crystal is a vacuum, the electromagnetic waves would not be completely confined to the photonic crystal. All of these make the physics of photonic crystals more abundant and more diversified and might lead to more practical applications.

One-dimensional photonic crystals are the simplest photonic crystals. A clear and comprehensive understanding of the physics in one-dimensional photonic crystals is a basis for further understanding of the physics in two or three-dimensional photonic crystals. So far the transfer matrix method (TMM) [5, 8, 9] has been a major theoretical tool for investigations on the simplest one-dimensional photonic crystals—a structure made of alternative layers of two different isotropic homogeneous dielectric materials. By this method, one solves the wave equations in each medium layer of a period unit, matches the relevant components of the magnetic field and electric field according to the necessary continuous conditions at the interfaces and then uses the Bloch theorem to treat the periodicity. Then the required results such as the dispersion
relation etc. can be obtained after unknown arbitrary constants were canceled [8, 9].
Much of our current fundamental theoretical understandings on one-dimensional photonic crystals made of two different dielectric media was mainly obtained from TMM.

The modern mathematical theory of periodic Sturm–Liouville equations can treat a one-dimensional layered photonic crystal as a whole, rather than each medium layer separately, since the matching conditions at each interface required by TMM are implicitly contained in the wave equations. In this Appendix, we apply the theory summarized in Chap. 2 to treat one-dimensional photonic crystals, in the order of infinite size, semi-infinite size, and finite size, to understand some of the fundamental physics of one-dimensional photonic crystals, including the physics closely related to the very existence of the boundary and boundaries.

Many authors working on photonic crystals compare electromagnetic waves with electronic waves in periodic systems to illustrate the physics of photonic crystals, see, for example, [12, 16–18, 21, 23]. By the modern theory of periodic Sturm–Liouville equations, the wave equations for electromagnetic waves in some one-dimensional photonic crystals and the Schrödinger equation for electronic states in one-dimensional electronic crystals are special cases of the more general periodic Sturm–Liouville equations. Such a comparison now has a clear theoretical basis. We will also see that some understandings we learned on the one-dimensional electronic crystals in Chaps. 3 and 4 have their analogs or correspondences in one-dimensional photonic crystals.

F.1 Wave Equations

We treat the simplest photonic crystals. We assume that the magnetic permeability of the photonic crystal is equal to that of free space \( \mu_0 \) and that the relative dielectric coefficient \( \varepsilon(x) \) is isotropic, real, periodic with \( x \), and does not depend on frequency. The Maxwell equations for the propagation of light in such a photonic crystal composed of a mixed homogeneous dielectric medium with no free charges or currents lead to four equations (in CGS units) [5, 8, 9, 12, 17]:

\[
\begin{align*}
\frac{1}{\varepsilon(x)} \nabla \times \nabla \times \mathbf{E}(x, t) &= -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{E}(x, t), \\
\nabla \times \left[ \frac{1}{\varepsilon(x)} \nabla \times \mathbf{H}(x, t) \right] &= -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{H}(x, t), \\
\nabla \cdot \varepsilon(x) \mathbf{E}(x, t) &= 0, \\
\nabla \cdot \mathbf{H}(x, t) &= 0.
\end{align*}
\]

(F.1)

Here, \( \mathbf{E}(x, t) \) and \( \mathbf{H}(x, t) \) are the electric field and magnetic field respectively, and \( c \) is the speed of light in free space.
We are interested in the solutions of (F.1) with the form

\[ E(x, t) = E(x) e^{-i\omega t}, \]
\[ H(x, t) = H(x) e^{-i\omega t}, \]

where \( \omega \) is the eigen-angular frequency, \( E(x) \) and \( H(x) \) are the eigenfunctions of the equations

\[ \frac{1}{\varepsilon(x)} \nabla \times \nabla \times E(x) - \left( \frac{\omega}{c} \right)^2 E(x) = 0, \]  

(F.2)

and

\[ \nabla \times \left[ \frac{1}{\varepsilon(x)} \nabla \times H(x) \right] - \left( \frac{\omega}{c} \right)^2 H(x) = 0. \]  

(F.3)

The electromagnetic wave modes in such a photonic crystal can be solved using (F.3) and

\[ \nabla \cdot H(x) = 0, \]  

(F.4)

then \( E(x) \) can be obtained from \( H(x) \) using

\[ \nabla \times H(x) - \frac{i \omega}{c} \varepsilon(x) E(x) = 0; \]  

(F.5)

Alternatively, they can also be solved by using (F.2) and

\[ \nabla \cdot \varepsilon(x) E(x) = 0, \]  

(F.6)

and \( H(x) \) can be obtained from \( E(x) \) using

\[ \nabla \times E(x) + \frac{i \omega}{c} \varepsilon(x) H(x) = 0. \]  

(F.7)

### F.2 TM Modes and TE Modes

In the following, we are interested in one-dimensional photonic crystals where \( \varepsilon(x) \) is only a function of \( x \), and it is a periodic function of \( x : \varepsilon(x + a) = \varepsilon(x) \).

We choose the plane of wave propagation as the \( xz \) plane. An electromagnetic wave propagating in the \( xz \) plane can be either a TM mode where the magnetic field \( H(x) \) is in the \( y \) direction or a TE mode where the electric field \( E(x) \) is in the \( y \) direction.
F.2.1 TM Modes

For a TM mode, the magnetic field $\mathbf{H}(x)$ is in the $y$ direction. $\mathbf{H}(x)$ can be written as

$$H_x = 0, \quad H_y = H_y(x)e^{ik_z z}, \quad H_z = 0.$$ 

Let $y(x) = H_y(x)$, from Eqs. (F.3) and (F.5) we obtain that for a TM mode

$$\left[ \frac{1}{\varepsilon(x)} y'(x) \right]' + \left( \frac{\omega}{c} \right)^2 - \frac{1}{\varepsilon(x)} k_z^2 \right] y(x) = 0, \quad (F.8)$$

and

$$E_x \frac{\omega}{c} \varepsilon(x) = -k_z y(x)e^{ik_z z}, \quad E_y = 0, \quad E_z \frac{i\omega}{c} \varepsilon(x) = y'(x)e^{ik_z z}. \quad (F.9)$$

Equation (F.8) is a specific form of Eq. (2.2) with $p(x) = \frac{1}{\varepsilon(x)}$, $q(x) = -\frac{1}{\varepsilon(x)} k_z^2$, $w(x) = \frac{1}{c}$ and $\lambda = \omega^2$. In the simplest one-dimensional photonic crystals—the layered photonic crystals,— $\varepsilon(x)$ is a piecewise continuous step function rather than a continuous function. Therefore, Eq. (F.8) is not a Hill’s equation in Eastham’s book [26]. This is the reason that in the previous edition of this book, it was stated that the theory of the Hill’s equations could not be used to treat photonic crystals. Nevertheless, the modern theory of periodic Sturm–Liouville equations summarized in Chap. 2 can be straightforward applied to treat Eq. (F.8) for layered photonic crystals.

By the mathematical theory, each solution $y$ of Eq. (F.8) and its quasi-derivative $\frac{1}{\varepsilon(x)} y'(x)$ are continuous. Thus, the requirements that $H_y$ and $E_z$ are continuous for a TM mode [5, 8, 9] are implicitly contained in Eqs. (F.8) and (F.9).

According to the theory in Chap. 2, the band structure of TM modes is determined by the discriminant $D_{tm}(\lambda)$ of Eq. (F.8) defined as

$$D_{tm}(\lambda) = \eta_1(a, \lambda) + \frac{1}{\varepsilon(a)} \eta_2'(a, \lambda), \quad (F.10)$$

where $\eta_1(x, \lambda)$ and $\eta_2(x, \lambda)$ are two linearly independent normalized solutions of Eq. (F.8) satisfying that

$$\eta_1(0, \lambda) = 1, \quad \frac{1}{\varepsilon(0)} \eta_1'(0, \lambda) = 0; \quad \eta_2(0, \lambda) = 0, \quad \frac{1}{\varepsilon(0)} \eta_2'(0, \lambda) = 1. \quad (F.11)$$

The permitted TM bands correspond to the $\lambda$ ranges where $-2 \leq D_{tm}(\lambda) \leq 2$. The band structure can be obtained from $D_{tm}(\lambda)$ in these ranges by (2.74) as

$$\cos k_x a = \frac{1}{2} D_{tm}(\lambda), \quad (F.12)$$

where $k_x$ is the Bloch wavevector: $-\frac{\pi}{a} < k_x \leq \frac{\pi}{a}$. 

**F.2.2 TE Modes**

For a TE mode, the electric field $\mathbf{E}(x)$ is in the y direction, and $\mathbf{E}(x)$ can be written as

$$ E_x = 0, \quad E_y = E_y(x)e^{ik_z z}, \quad E_z = 0. $$

Let $y = E_y(x)$, from Eqs. (F.2) and (F.7) we obtain that for a TE Mode

$$ y''(x) + \left[ \varepsilon(x) \left( \frac{\omega}{c} \right)^2 - k_z^2 \right] y(x) = 0, \quad (F.13) $$

and

$$ H_x \frac{\omega}{c} = k_z y(x)e^{ik_z z}, \quad H_y = 0, \quad H_z \frac{i\omega}{c} = -y'(x)e^{ik_z z}. \quad (F.14) $$

Equation (F.13) is a special case of Eq. (2.2) with $p(x) = 1, q(x) = k_z^2, w(x) = \varepsilon(x)(\frac{1}{c^2})$ and $\lambda = \omega^2$. The mathematical theory in Chap. 2 can be applied to Eq. (F.13). The requirements of $E_y$ and $H_z$ being continuous for a TE mode [5, 8, 9] are implicitly contained in Eqs. (F.13) and (F.14), since each solution $y$ of Eq. (F.8) and its derivative $y'$ are continuous.

According to the theory of Chap. 2, the band structure of TE modes is determined by the discriminant $D_{te}(\lambda)$ of Eq. (F.13) defined as

$$ D_{te}(\lambda) = \eta_1(a, \lambda) + \eta_2^2(a, \lambda), \quad (F.15) $$

where $\eta_1(x, \lambda)$ and $\eta_2(x, \lambda)$ are two linearly independent normalized solutions of Eq. (F.13) satisfying that

$$ \eta_1(0, \lambda) = 1, \quad \eta_1'(0, \lambda) = 0; \quad \eta_2(0, \lambda) = 0, \quad \eta_2'(0, \lambda) = 1. \quad (F.16) $$

The permitted TE bands correspond to the ranges of $\lambda$ where $-2 \leq D_{te}(\lambda) \leq 2$. The band structure can be obtained from $D_{te}(\lambda)$ in each range by (2.74) as

$$ \cos k_x a = \frac{1}{2} D_{te}(\lambda), \quad (F.17) $$

where $k_x$ is the Bloch wavevector: $-\frac{\pi}{a} < k_x \leq \frac{\pi}{a}$.

**F.2.3 Band Structures of a One-Dimensional Layered Photonic Crystal Made of Two Different Materials**

The simplest cases are where a one-dimensional photonic crystal is made of two different dielectric materials with dielectric constants $\varepsilon_1, \varepsilon_2$ and thicknesses $d_1, d_2$ alternatively.
F.2.3.1 TM Modes

In such a layered photonic crystal, Eq. (F.8) can be written as

\[
\left[ \frac{1}{\varepsilon_l} y'(x) \right]' + \left[ \frac{\lambda}{c^2} - \frac{k_2^2}{\varepsilon_l} \right] y(x) = 0, \quad (F.18)
\]

where

\[
\varepsilon_l = \begin{cases} 
\varepsilon_1, & na < x \leq d_1 + na, \\
\varepsilon_2, & na + d_1 < x \leq (n+1)a.
\end{cases} \quad (F.19)
\]

Here \( \lambda = \omega^2 \geq 0 \), \( a = d_1 + d_2 \) is the period, \( n \) is an integer and \( \varepsilon_1 \neq \varepsilon_2 \) are positive real constants. Equation (F.18) corresponds to a special case of (2.2) where \( p(x) = \frac{1}{\varepsilon_l} \) and \( q(x) = \frac{1}{c^2} k_2^2 \) are discontinuous at isolated points \( x = na \) and \( x = d_1 + na \), \( w(x) = \frac{1}{\varepsilon_l} > 0 \).

Equation (F.18) can be rewritten as

\[
\left[ \frac{1}{\varepsilon_l} y'(x) \right]' + \frac{1}{\varepsilon_l} k_l^2 y(x) = 0, \quad (F.20)
\]

where

\[
\frac{1}{\varepsilon_l} k_l^2 = \frac{\lambda}{c^2} - \frac{k_2^2}{\varepsilon_l}. \quad (F.21)
\]

Here \( k_l \) is real if \( \frac{\lambda}{c^2} - \frac{k_2^2}{\varepsilon_l} > 0 \) or imaginary if \( \frac{\lambda}{c^2} - \frac{k_2^2}{\varepsilon_l} < 0 \).

According to the theory in Chap. 2, the complex energy band structure—in both permitted bands and forbidden ranges—of the TM modes in a one-dimensional photonic crystal can be completely determined by the discriminant \( D_{tm}(\lambda) \) of the Eq. (F.18). By (C.31) in Appendix C, it is

\[
D_{tm}(\lambda) = 2 \cos k_2 d_2 \cos k_1 d_1 - \left[ \frac{k_1 \varepsilon_2}{k_2 \varepsilon_1} + \frac{k_2 \varepsilon_1}{k_1 \varepsilon_2} \right] \sin k_2 d_2 \sin k_1 d_1. \quad (F.22)
\]

As \( \lambda \) increases, \( D_{tm}(\lambda) \) changes in a way as \( D(\lambda) \) described in Sect. 2.4.

Most previous theoretical investigations on TM modes in photonic crystals are of their permitted band structure where \(-2 \leq D_{tm}(\lambda) \leq +2\). From (F.12) and (F.22) we obtain that for such a layered photonic crystal, the permitted band structure of TM modes is determined by

\[
\cos k_x a = \cos k_2 d_2 \cos k_1 d_1 - \frac{1}{2} \left[ \frac{k_1 \varepsilon_2}{\varepsilon_1 k_2} + \frac{k_2 \varepsilon_1}{\varepsilon_2 k_1} \right] \sin k_2 d_2 \sin k_1 d_1. \quad (F.23)
\]
Equation (F.23) essentially is the dispersion relation obtained in Sect. 6.2 in [8] and Sect. 6.2 in [9] and frequently seen in the literature, such as in [4, 27–31], etc.

The solutions in forbidden ranges where \(|D_{tm}(\lambda)| > 2\) are important for semi-infinite and finite photonic crystals, their behaviors also depend on \(D_{tm}(\lambda)\).

### F.2.3.2 TE Modes

For TE modes in such a layered photonic crystal, Eq. (F.13) can be written as

\[
y''(x) + \left[\frac{\lambda}{c^2} \varepsilon_l - k_z^2 \right] y(x) = 0, \tag{F.24}
\]

where

\[
\varepsilon_l = \begin{cases} 
\varepsilon_1, & na < x \leq d_1 + na, \\
\varepsilon_2, & na + d_1 < x \leq (n + 1). 
\end{cases} \tag{F.25}
\]

Here \(\lambda = \omega^2 \geq 0\), \(a = d_1 + d_2\) is the period, \(n\) is an integer, and \(\varepsilon_1 \neq \varepsilon_2\) are positive real constants. Equation (F.24) corresponds to a special case of Eq. (2.2) where \(p(x) = 1\), \(q(x) = k_z^2\), and \(w(x) = \frac{k_2^2}{\varepsilon_2} > 0\).

Equation (F.24) can be rewritten as

\[
y''(x) + k_l^2 y(x) = 0, \quad l = 1, 2, \tag{F.26}
\]

where

\[
k_l^2 = \frac{\lambda}{c^2} \varepsilon_l - k_z^2. \tag{F.27}
\]

Here \(k_l\) is real if \(\frac{\lambda}{c^2} \varepsilon_l - k_z^2 > 0\) or imaginary if \(\frac{\lambda}{c^2} \varepsilon_l - k_z^2 < 0\).

According to the theory in Chap. 2, the complex energy band structure—in both permitted bands and forbidden ranges—of the TE modes in the one-dimensional photonic crystal can be completely determined by the discriminant \(D_{te}(\lambda)\) of Eq. (F.24). By (C.31) in Appendix C, it is

\[
D_{te}(\lambda) = 2 \cos k_2 d_2 \cos k_1 d_1 - \left[\frac{k_1}{k_2} + \frac{k_2}{k_1}\right] \sin k_2 d_2 \sin k_1 d_1. \tag{F.28}
\]

As \(\lambda\) increases, \(D_{te}(\lambda)\) changes in the way as \(D(\lambda)\) described in Sect. 2.4.

Most previous theoretical investigations on TE modes in photonic crystals are of their permitted band structure where \(-2 \leq D_{te}(\lambda) \leq +2\). From (F.17) and (F.28) we can obtain that for such a layered photonic crystal, the permitted band structure of TE modes is determined by
\[
\cos k_x a = \cos k_2 d_2 \cos k_1 d_1 - \frac{1}{2} \left[ \frac{k_1}{k_2} + \frac{k_2}{k_1} \right] \sin k_2 d_2 \sin k_1 d_1. \quad \text{(F.29)}
\]

Equation (F.29) essentially is the dispersion relation obtained in Sect. 6.2 in [8] and Sect. 6.2 in [9] and frequently seen in the literature, such as in [4, 27–31], etc.

Theorem 2.7 gives the exact number of zeros of each band-edge mode. An eigenmode at the bottom or the top of the lowest band gap has exactly one zero in one period \(a\). Those are the facts shown in Fig. 3 in Chap. 4 of [12] and Figs. 3 and 4 in Chap. 4 of [17].

The solutions in forbidden ranges where \(|D_{te}(\lambda)| > 2\) are important for semi-infinite and finite photonic crystals, and their behaviors also depend on \(D_{te}(\lambda)\).

### F.2.4 Band Structure of a One-Dimensional Layered Photonic Crystal Made of More Different Materials

From above discussions, we have seen that an essential step for obtaining the band structures of a one-dimensional photonic crystal is to obtain the discriminants \(D_{tm}(\lambda)\) and \(D_{te}(\lambda)\). For a one-dimensional layered photonic crystal in which each unit cell is made of three or more different materials [32–35], the discriminant \(D_{tm}(\lambda)\) of Eq. (F.8) for TM modes and the discriminant \(D_{te}(\lambda)\) of Eq. (F.13) for TE modes can be obtained from relevant expressions in Appendix C.

#### F.2.4.1 TM Modes

For a one-dimensional layered photonic crystal in which each unit cell is made of three different homogeneous and isotropic dielectric materials with dielectric constants \(\varepsilon_1, \varepsilon_2, \varepsilon_3\) and thicknesses \(d_1, d_2, d_3\) alternatively, the band structure of TM modes can be obtained from (C.38) as

\[
\cos k_x a = \cos k_3 d_3 \cos k_2 d_2 \cos k_1 d_1 - \frac{1}{2} \left( \frac{\varepsilon_2 k_1}{\varepsilon_1 k_2} + \frac{\varepsilon_1 k_2}{\varepsilon_2 k_1} \right) \cos k_3 d_3 \sin k_2 d_2 \sin k_1 d_1 \\
- \frac{1}{2} \left( \frac{\varepsilon_3 k_1}{\varepsilon_1 k_3} + \frac{\varepsilon_1 k_3}{\varepsilon_3 k_1} \right) \sin k_3 d_3 \cos k_2 d_2 \sin k_1 d_1 \\
- \frac{1}{2} \left( \frac{\varepsilon_3 k_2}{\varepsilon_2 k_3} + \frac{\varepsilon_2 k_3}{\varepsilon_3 k_2} \right) \sin k_3 d_3 \sin k_2 d_2 \cos k_1 d_1. \quad \text{(F.30)}
\]

Here \(k_l, l = 1, 2, 3\) are given by

\[
\frac{1}{\varepsilon_l} k_l^2 = \frac{\lambda}{c^2} - \frac{k^2}{\varepsilon_l}, \quad \text{(F.31)}
\]

similarly as in Eq. (F.21).
For a one-dimensional layered photonic crystal in which each unit cell is made of four different homogeneous and isotropic dielectric materials, the discriminant $D_{tm}(\lambda)$ of Eq. (F.8) can be obtained in (C.43). The band structure can be obtained accordingly from (C.44). If needed, for a one-dimensional layered photonic crystal in which each unit cell is made of five or more different homogeneous and isotropic dielectric materials, the discriminant $D_{tm}(\lambda)$ of Eq. (F.8) can be obtained similarly by using the approach in Appendix C. The band structure can be obtained accordingly.

F.2.4.2 TE Modes

For a one-dimensional layered photonic crystal in which each unit cell is made of three different homogeneous and isotropic dielectric materials, the band structure of TE modes can be obtained from (C.38) as

$$\cos k_3 a = \cos k_3 d_3 \cos k_2 d_2 \cos k_1 d_1$$
$$-\frac{1}{2} \left( \frac{k_1}{k_2} + \frac{k_2}{k_1} \right) \cos k_3 d_3 \sin k_2 d_2 \sin k_1 d_1$$
$$-\frac{1}{2} \left( \frac{k_1}{k_3} + \frac{k_3}{k_1} \right) \sin k_3 d_3 \cos k_2 d_2 \sin k_1 d_1$$
$$-\frac{1}{2} \left( \frac{k_2}{k_3} + \frac{k_3}{k_2} \right) \sin k_3 d_3 \sin k_2 d_2 \cos k_1 d_1. \quad (F.32)$$

Here $k_l, l = 1, 2, 3$ are given by

$$k_l^2 = \frac{\lambda}{c^2} \varepsilon_l - k_z^2, \quad (F.33)$$

similarly as in Eq. (F.27).

Similarly, for a one-dimensional layered photonic crystal in which each unit cell is made of four different homogeneous and isotropic dielectric materials, the discriminant $D_{te}(\lambda)$ of Eq. (F.13) can be obtained from (C.43). The band structure can be obtained accordingly from (C.44). If needed, for a one-dimensional layered photonic crystal in which each unit cell is made of five or more different homogeneous and isotropic dielectric materials, the discriminant $D_{tm}(\lambda)$ of Eq. (F.13) can also be obtained similarly by using the approach in Appendix C, and the band structure can be obtained accordingly.

F.3 Surface Modes in Semi-infinite One-Dimensional Photonic Crystals

A semi-infinite one-dimensional photonic crystal may have surface modes existing in band gaps and localized near the boundary surface. There have been interesting
investigations on surface modes in one-dimensional photonic crystals in the literature, see, for example, [7–9, 12, 18, 27–31, 36–50] and references therein. As in cases of infinite one-dimensional photonic crystals, a previous primary theoretical tool is the transfer matrix method. Many interesting results and fundamental understandings of the surface modes in semi-infinite one-dimensional photonic crystals were obtained by this method.

In this section, we use the theory of periodic Sturm–Liouville equations in Chap. 2 to treat the problem. A general formalism of theoretical investigations on the surface modes in one-dimensional photonic crystals can be developed, and new fundamental understandings can be obtained.

The surface modes in a one-dimensional semi-infinite photonic crystal, in general, are different from the surface states in an ideal semi-infinite electronic crystal, or a semi-infinite phononic crystal with a free boundary surface: The electromagnetic waves are not completely confined to the semi-infinite photonic crystal even where the medium outside of a photonic crystal is a vacuum. Because of this, the surface modes in a one-dimensional semi-infinite photonic crystal can only exist below the light line such as shown in Fig. 13 of Chap. 4 in [12] or Fig. 14 of Chap. 4 in [17].

### F.3.1 Surface TM Modes

For a simple semi-infinite one-dimensional photonic crystal with an external homogeneous medium of a dielectric constant $\varepsilon_0 > 0$ at the left boundary $\tau$, the wave equation for the TM modes can be written as

$$\left[ \frac{1}{\varepsilon(x)} \psi'(x) \right]' + \left[ \left( \frac{\Omega}{c} \right)^2 - \frac{1}{\varepsilon(x)} k_z^2 \right] \psi(x) = 0, \quad x > \tau, \quad (F.34)$$

in the photonic crystal and

$$\psi''(x) + \left[ \varepsilon_0 \left( \frac{\Omega}{c} \right)^2 - k_z^2 \right] \psi(x) = 0, \quad x < \tau, \quad (F.35)$$

in the external medium, with conditions that $H_y$ and $E_z$ are continuous at $\tau$.

A solution of Eq. (F.35) can be decaying in the $-x$ direction only when $\varepsilon_0 \left( \frac{\Omega}{c} \right)^2 - k_z^2 < 0$. That is, a localized surface mode can only exist if it is below the light line $\omega = \frac{c}{\sqrt{\varepsilon_0}} k_z$. Equation (F.35) can be solved for a constant $\varepsilon_0$ as

$$\psi(x) = Ce^{\gamma x}, \quad x < \tau, \quad (F.36)$$
where
\[
\gamma = \left[ k_z^2 - \varepsilon_0 \left( \frac{\Omega}{c} \right)^2 \right]^{1/2} > 0. \tag{F.37}
\]

By considering the continuous conditions of \( H_y \) and \( E_z \) for TM modes at the boundary \( \tau \), the wave equation inside the photonic crystal can now be written in the form of
\[
\left[ \frac{1}{\varepsilon(x)} \psi'(x) \right]' + \left[ \left( \frac{\Omega}{c} \right)^2 - \frac{1}{\varepsilon(x)} k_z^2 \right] \psi(x) = 0, \quad x > \tau, \tag{F.38}
\]
where
\[
\sigma_{tm} = \frac{1}{\varepsilon_0} \left[ k_z^2 - \varepsilon_0 \left( \frac{\Omega}{c} \right)^2 \right]^{1/2} \tag{F.39}
\]
is a quantity determined by \( \Omega, k_z \) and \( \varepsilon_0 \).\(^{10}\)

We are only interested in the solutions of Eq. (F.38) which are localized near the boundary \( \tau \). From Sect. 2.5 in Chap. 2, we know that if a solution of Eq. (F.34) localized near \( \tau \) exists, it is in a band gap of Eq. (F.8). Such a solution has the form
\[
\psi(x, \Lambda) = e^{-\beta(\Lambda)x} f(x, \Lambda), \tag{F.40}
\]
where \( \beta(\Lambda) > 0 \). Here \( f(x, \Lambda) \) is a periodic function \( p(x + a, \Lambda) = p(x, \Lambda) \) if the band-gap is located at the center of the Brillouin zone \( k_x = 0 \), or a semi-periodic function \( s(x + a, \Lambda) = -s(x, \Lambda) \) if the band-gap is located at the boundary of the Brillouin zone \( k_x = \pi a \). Consequently, the following equation is a necessary condition for the existence of such a surface mode:
\[
\sigma_{tm} \psi(\tau + a, \Lambda) - \frac{1}{\varepsilon(\tau)} \psi'(\tau + a, \Lambda) = \sigma_{tm} \psi(\tau, \Lambda) - \frac{1}{\varepsilon(\tau)} \psi'(\tau, \Lambda) = 0. \tag{F.41}
\]

Any solution \( \psi \) of Eqs. (F.34) and (F.35) or Eq. (F.38) in the semi-infinite crystal \( x \geq \tau \) can be expressed as a linear combination of two normalized solutions of Eq. (F.8):
\[
\psi(x, \lambda) = c_1 \eta_1(x, \lambda) + c_2 \eta_2(x, \lambda), \quad x \geq \tau, \tag{F.42}
\]

\(^{10}\)Since for a TM mode, \( H_y \) and \( E_z \) are continuous, from Eq. (F.9) one can obtain that \( \psi_{\tau-0} = \psi_{\tau+0} \) and \( \frac{\psi'_{\tau-0}}{\varepsilon_0} = \frac{\psi'_{\tau+0}}{\varepsilon(\tau)} \). Thus \( \sigma_{tm} = \frac{\psi'_{\tau+0}}{\varepsilon(\tau)\psi_{\tau+0}} = \frac{\psi'_{\tau-0}}{\varepsilon_0 \psi_{\tau-0}} = \frac{\gamma}{\varepsilon_0} \).
where \( \eta_1(x, \lambda) \) and \( \eta_2(x, \lambda) \) are two linearly independent solutions of Eq. (F.8) defined by

\[
\eta_1(\tau, \lambda) = 1, \quad \frac{1}{\varepsilon(\tau)} \eta_1'(\tau, \lambda) = 0; \quad \eta_2(\tau, \lambda) = 0, \quad \frac{1}{\varepsilon(\tau)} \eta_2'(\tau, \lambda) = 1. \quad (F.43)
\]

From Eqs. (F.41), (F.42) and (F.43), a reasoning similar to Sect. 3.5 or E.2.2 leads to that the existence and properties of a TM surface mode in a one-dimensional semi-infinite photonic crystal are determined by the following two equations:

\[
\frac{1}{\varepsilon_0} \left[ k_z^2 - \frac{\Omega^2}{c^2} \right]^{1/2} = -\eta_1(\tau + a, \Omega^2) + \frac{1}{\varepsilon(\tau)} \eta_2'(\tau + a, \Omega^2) + \sqrt{D_{tm}(\Omega^2) - 4 \eta_2'(\tau + a, \Omega^2)} \quad (F.44)
\]

for a band gap at \( k_x = \pi/a \), or

\[
\frac{1}{\varepsilon_0} \left[ k_z^2 - \frac{\Omega^2}{c^2} \right]^{1/2} = -\eta_1(\tau + a, \Omega^2) + \frac{1}{\varepsilon(\tau)} \eta_2'(\tau + a, \Omega^2) - \sqrt{D_{tm}(\Omega^2) - 4 \eta_2'(\tau + a, \Omega^2)} \quad (F.45)
\]

for a band gap at \( k_x = 0 \). These two equations can be used to investigate how the existence of a surface TM mode and its properties in a specific one-dimensional semi-infinite photonic crystal depend on the boundary location \( \tau \) and the external medium.

More specifically, for the simple cases where a one-dimensional photonic crystal is alternatively made of two different dielectric media, without losing generality, we can consider only the cases where the surface boundary \( \tau \) is in the medium 1, thus, \( 0 \leq \tau \leq d_1 \).

The simplest cases are that the boundary layer is a full layer of medium 1, thus, \( \tau = 0 \). The existence and properties of a surface TM mode are determined by Eqs. (F.44) and (F.45) where

\[
\eta_1(\tau + a, \lambda) = \cos k_2d_2 \cos k_1d_1 - \frac{k_1 \varepsilon_2}{k_2 \varepsilon_1} \sin k_2d_2 \sin k_1d_1,
\]

\[
\eta_2(\tau + a, \lambda) = \frac{\varepsilon_1}{k_1} \cos k_2d_2 \sin k_1d_1 + \frac{\varepsilon_2}{k_2} \sin k_2d_2 \cos k_1d_1,
\]

\[
\frac{1}{\varepsilon(\tau)} \eta_2'(a, \lambda) = \cos k_2d_2 \cos k_1d_1 - \frac{k_2 \varepsilon_1}{k_1 \varepsilon_2} \sin k_2d_2 \sin k_1d_1. \quad (F.46)
\]

as given in (C.27), (C.29) and (C.30) and \( D_{tm}(\lambda) \) is given in (F.22).

In more general cases where \( \tau \neq 0 \), the photonic crystal made of two media can be seen as a particular case of a photonic crystal made of three media with dielectric constants \( \varepsilon_1, \varepsilon_2, \varepsilon_3 \) and thicknesses of \( d_1 - \tau, d_2, \tau \). We can now treat the boundary \( \tau \) as the origin of the three-media photonic crystal by defining \( \eta_1(x, \lambda) \) and \( \eta_2(x, \lambda) \) as in (F.43). From Eqs. (C.33), (C.35) and (C.36) we can obtain that
\[
\eta_1(\tau + a, \lambda) = \cos k_2 d_2 \cos k_1 d_1 - \sin k_2 d_2 \left[ \frac{\varepsilon_2 k_1}{\varepsilon_1 k_2} \sin k_1 (d_1 - \tau) \cos k_1 \tau + \frac{\varepsilon_1 k_2}{\varepsilon_2 k_1} \cos k_1 (d_1 - \tau) \sin k_1 \tau \right],
\]
\[
\eta_2(\tau + a, \lambda) = \frac{\varepsilon_1}{k_1} \cos k_2 d_2 \sin k_1 d_1 + \frac{\varepsilon_2}{k_2} \sin k_2 d_2 \cos k_1 d_1
\]
\[
+ \frac{\varepsilon_2}{k_2} \left( 1 - \frac{\varepsilon_1^2 k_2^2}{\varepsilon_2^2 k_1^2} \right) \sin k_2 d_2 \sin k_1 (d_1 - \tau) \sin k_1 \tau,
\]
\[
\frac{1}{\varepsilon(\tau)} \eta_2'(\tau + a, \lambda) = \cos k_2 d_2 \cos k_1 d_1 - \sin k_2 d_2 \left[ \frac{\varepsilon_1 k_2}{\varepsilon_2 k_1} \sin k_1 (d_1 - \tau) \cos k_1 \tau + \frac{\varepsilon_2 k_1}{\varepsilon_1 k_2} \cos k_1 (d_1 - \tau) \sin k_1 \tau \right],
\]
(F.47)

which can be used in Eq. (F.44) or (F.45) with \( D_{tm}(\lambda) \) given in (F.22).

For cases where a one-dimensional photonic crystal is made alternatively of three different dielectric media, without losing generality, we can also consider only the cases where the boundary \( \tau \) is in the medium 1 thus we have \( 0 \leq \tau \leq d_1 \). The photonic crystal made of three media can be seen as a particular case of a photonic crystal made of four media with the dielectric constants \( \varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_1 \) and the thickness of \( d_1 - \tau, d_2, d_3, \tau \). We can now treat the boundary \( \tau \) as the origin of the four-media photonic crystal by defining \( \eta_1(x, \lambda) \) and \( \eta_2(x, \lambda) \) as in (F.43). From Eqs. (C.39), (C.41) and (C.42) we can obtain \( \eta_1(\tau + a, \lambda), \eta_2(\tau + a, \lambda), \frac{1}{\varepsilon(\tau)} \eta_2'(\tau + a, \lambda) \) which can be used in Eqs. (F.44) or (F.45) with \( D_{tm}(\lambda) \) given in (C.37).

### F.3.2 Surface TE Modes

For a simple semi-infinite one-dimensional photonic crystal with an external homogeneous medium of a dielectric constant \( \varepsilon_0 > 0 \) at the left boundary \( \tau \), the wave equation for the TE modes can be written as

\[
\psi''(x) + \left[ \varepsilon(x) \left( \frac{\Omega c}{c} \right)^2 - k_\perp^2 \right] \psi(x) = 0, \quad x > \tau,
\]
(F.48)

and

\[
\psi''(x) + \left[ \varepsilon_0 \left( \frac{\Omega c}{c} \right)^2 - k_\perp^2 \right] \psi(x) = 0, \quad x < \tau,
\]
(F.49)

with the conditions that \( E_y \) and \( H_\perp \) are continuous at \( \tau \).

A solution of Eq. (F.49) can be decaying in the \(-x\) only when \( \varepsilon_0 \left( \frac{\Omega c}{c} \right)^2 - k_\perp^2 < 0 \).

That is, a localized surface mode can only exist if it is below the light line \( \omega = \frac{\sqrt{\varepsilon_0}}{k_\perp} \).
Equation (F.49) can be solved for a constant $\varepsilon_0$ as

$$\psi(x) = Ce^{\gamma x}, \quad x < \tau,$$

where

$$\gamma = \left[ k_z^2 - \varepsilon_0 \left( \frac{\Omega}{c} \right)^2 \right]^{1/2} > 0.$$ (F.51)

By considering the continuous conditions of $E_y$ and $H_z$ at the boundary $\tau$, the wave equation inside the photonic crystal can now be written in the form of

$$\psi''(x) + \left[ \varepsilon(x) \left( \frac{\Omega}{c} \right)^2 - k_z^2 \right] \psi(x) = 0, \quad x > \tau,$$

$$\sigma_{te} \psi(x) = \psi'(x), \quad x = \tau + 0,$$ (F.52)

where

$$\sigma_{te} = \left[ k_z^2 - \varepsilon_0 \left( \frac{\Omega}{c} \right)^2 \right]^{1/2}.$$ (F.53)

is a quantity determined by $\Omega$, $k_z$ and $\varepsilon_0$.\(^\text{11}\)

We are only interested in the solutions of (F.52) which are localized near the boundary $\tau$. From Sect. 2.5 in Chap. 2, we can see that if a solution of Eq. (F.48) localized near $\tau$, it is in a band gap of (F.13). Such a solution has the form

$$\psi(x, \Lambda) = e^{-\beta(\Lambda)x} f(x, \Lambda),$$ (F.54)

where $\beta(\Lambda) > 0$. Here $f(x, \Lambda)$ is either a periodic function $p(x + a, \Lambda) = p(x, \Lambda)$ if the band-gap is situated at the center of the Brillouin zone $k_x = 0$ or a semi-periodic function $s(x + a, \Lambda) = -s(x, \Lambda)$ if the band-gap is situated at the boundary of the Brillouin zone $k_x = \frac{\pi}{a}$.

Consequently, the following equation is a necessary condition for the existence of such a surface mode:

$$\sigma_{te} \psi(\tau + a, \Lambda) - \psi'(\tau + a, \Lambda) = \sigma_{te} \psi(\tau, \Lambda) - \psi'(\tau, \Lambda) = 0.$$ (F.55)

Any solution $\psi$ of Eqs. (F.48) and (F.49) or Eq. (F.52) for $\tau > 0$ can be expressed as a linear combination of two normalized solutions of Eq. (F.24):

$$\psi(x, \lambda) = c_1 \eta_1(x, \lambda) + c_2 \eta_2(x, \lambda), \quad x \geq \tau,$$ (F.56)

\(^{11}\)Since for a TE mode, $E_y$ and $H_z$ are continuous, from Eq. (F.14) one obtains that $\psi_{\tau-0} = \psi_{\tau+0}$ and $\psi'_{\tau-0} = \psi'_{\tau+0}$. Thus $\sigma_{te} = \frac{\psi'_{\tau+0}}{\psi_{\tau+0}} = \frac{\psi'_{\tau-0}}{\psi_{\tau-0}} = \gamma$. 

where \( \eta_1(x, \lambda) \) and \( \eta_2(x, \lambda) \) are two linearly independent solutions of Eq. (F.24) defined by

\[
\eta_1(\tau, \lambda) = 1, \quad \eta_1'(\tau, \lambda) = 0; \quad \eta_2(\tau, \lambda) = 0, \quad \eta_2'(\tau, \lambda) = 1.
\]  

From Eqs. (F.55), (F.56) and (F.57), the reasonings similar to Sect. 3.5 or E.2.2 give that the existence and properties of a TE surface mode in a one-dimensional semi-infinite photonic crystal are determined by the following two equations:

\[
\left[ k_z^2 - \varepsilon_0 \left( \frac{\Omega}{c} \right)^2 \right]^{1/2} = -\eta_1(\tau + a, \Omega^2) + \eta_2(\tau + a, \Omega^2) + \sqrt{D_{te}(\Omega^2) - 4} \over 2 \eta_2(\tau + a, \Omega^2), \quad (F.58)
\]

for a band gap at \( k_x = \pi/a \) or

\[
\left[ k_z^2 - \varepsilon_0 \left( \frac{\Omega}{c} \right)^2 \right]^{1/2} = -\eta_1(\tau + a, \Omega^2) + \eta_2(\tau + a, \Omega^2) - \sqrt{D_{te}(\Omega^2) - 4} \over 2 \eta_2(\tau + a, \Omega^2), \quad (F.59)
\]

for a band gap at \( k_x = 0 \). These two equations can be used to investigate how the existence of a surface TE mode and its properties in a specific one-dimensional semi-infinite photonic crystal depend on the boundary \( \tau \) and the external medium.

More specifically, for the simple cases where a one-dimensional photonic crystal is made of two different dielectric media alternatively, without losing generality, we can consider only the cases where the boundary \( \tau \) is in the medium 1, thus, \( 0 \leq \tau \leq d_1 \).

The simplest cases are where the boundary layer is a full layer of medium 1 thus \( \tau = 0 \), the existence and properties of a surface mode are determined by Eqs. (F.58) or (F.59) where

\[
\eta_1(\tau + a, \lambda) = \cos k_2 d_2 \cos k_1 d_1 - \frac{k_1}{k_2} \sin k_2 d_2 \sin k_1 d_1,
\]

\[
\eta_2(\tau + a, \lambda) = \frac{1}{k_1} \cos k_2 d_2 \sin k_1 d_1 + \frac{1}{k_2} \sin k_2 d_2 \cos k_1 d_1,
\]

\[
\eta_2'(\tau + a, \lambda) = \cos k_2 d_2 \cos k_1 d_1 - \frac{k_2}{k_1} \sin k_2 d_2 \sin k_1 d_1.
\]  

as given in (C.27), (C.29) and (C.30). \( D_{te}(\lambda) \) is given in (F.28). The equations obtained are essentially same as equations previously obtained for the existence of TE surface modes such as Eqs. (6.9)–(5) in [8], Eqs. (11.5)–(6) in [9] and used in [30].

In more general cases where \( \tau \neq 0 \), the photonic crystal made of two media can be considered as a particular case of a photonic crystal made of three media with dielectric constants \( \varepsilon_1, \varepsilon_2, \varepsilon_1 \), and thicknesses of \( d_1 - \tau, d_2, \tau \). We can now treat the boundary \( \tau \) as the origin of the three-media photonic crystal by defining \( \eta_1(x, \lambda) \) and \( \eta_2(x, \lambda) \) as (F.57). From Eqs. (C.33), (C.35) and (C.36), we obtain that
\[ \eta_1(\tau + a, \lambda) = \cos k_2 d_2 \cos k_1 d_1 \]
\[-\sin k_2 d_2 \left[ \frac{k_1}{k_2} \sin k_1 (d_1 - \tau) \cos k_1 \tau + \frac{k_2}{k_1} \cos k_1 (d_1 - \tau) \sin k_1 \tau \right], \]
\[ \eta_2(\tau + a, \lambda) = \frac{1}{k_1} \cos k_2 d_2 \sin k_1 d_1 + \frac{1}{k_2} \sin k_2 d_2 \cos k_1 d_1 \]
\[+ \frac{1}{k_2} \left( 1 - \frac{k_2^2}{k_1^2} \right) \sin k_2 d_2 \sin k_1 (d_1 - \tau) \sin k_1 \tau, \]
\[ \eta_2'(\tau + a, \lambda) = \cos k_2 d_2 \cos k_1 d_1 \]
\[-\sin k_2 d_2 \left[ \frac{k_2}{k_1} \sin k_1 (d_1 - \tau) \cos k_1 \tau + \frac{k_1}{k_2} \cos k_1 (d_1 - \tau) \sin k_1 \tau \right], \] (F.61)

which can be used in Eq. (F.58) or (F.59) with \( D_{te}(\lambda) \) given in (F.28).

For cases where a one-dimensional photonic crystal is made alternatively of three different dielectric media, without losing generality, we can also consider only the cases where the surface boundary is in the medium 1, thus, \( 0 \leq \tau \leq d_1 \). The photonic crystal made of three media can be considered as a particular case of a photonic crystal made of four media with dielectric constants \( \varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4 \), and thickness \( d_1 - \tau, d_2, d_3, \tau \). We can now treat the boundary \( \tau \) as the origin of the four-media photonic crystal by defining \( \eta_1(x, \lambda) \) and \( \eta_2(x, \lambda) \) as in (F.57). From Eqs. (C.39), (C.41) and (C.42) we can obtain \( \eta_1(\tau + a, \lambda), \eta_2(\tau + a, \lambda), \eta_2'(\tau + a, \lambda) \) which can be used in Eq. (F.58) or (F.59) with \( D_{te}(\lambda) \) given in (C.37).

### F.3.3 Discussions

A major theoretical formalism widely used in previous investigations on surface modes in one-dimensional photonic crystals such as [8, 9, 30] treated the simplest one-dimensional photonic crystals made of two media and the outmost layer is a whole layer of one medium. Previous theoretical investigations on surface modes with different surface termination locations used a super-cell method such as in [37, 38] or other numerical methods [12, 17]. The theoretical formalism developed in Sects. F.3.1 and F.3.2 is more general and easy to use. As a simple example, in Fig.F.1 is shown the surface band structure of a semi-infinite one-dimensional photonic crystal investigated in [12, 17], with more different surface termination locations. Note that the \( \tau \)-regions where the TE surface bands exist are different for different bulk band gaps. In each bulk band gap, as the boundary goes inside—that is, as \( \tau \) increases—, the surface band curve goes higher.

In this section, we only treated surface modes in semi-infinite photonic crystals (without a cap layer) for simplicity. A slightly extended formalism can be developed to treat surface modes in semi-infinite photonic crystals with a cap layer, where the left side in Eqs. (F.44) and (F.45) or Eqs. (F.58) and (F.59) will be mathematical expressions containing parameters of the cap layer such as thickness, dielectric coefficient, and so forth.
Appendix F: One-Dimensional Photonic Crystals

Fig. F.1 Change of TE surface band structure of a semi-infinite one-dimensional photonic crystal investigated in [12, 17] as the surface location $\tau$ changes. The one-dimensional photonic crystal is the same as the one in Fig. 13 of Chap. 4 in [12] and Fig. 14 of Chap. 4 in [17]. The outmost layer is an $\varepsilon = 13$ layer, with a layer thickness $0.2a - \tau$. The solid (dashed) lines are band edges at $k_x = 0 (k_x = \frac{\pi}{a})$ of the bulk bands. The thin solid line is the light line. Each one-dot chained line corresponds to a surface band in the lowest bulk band gap at $k_x = \frac{\pi}{a}$ obtained from (F.58). The chained line of $\tau = 0.1a$ in the figure corresponds to the surface band structure in the mentioned figures in [12, 17]. Each two-dot chained line corresponds to a surface band in the lowest bulk band gap at $k_x = 0$ obtained from (F.59).

The theoretical formalisms developed in Sects. F.3.1 and F.3.2 can be extended to investigate evanescent modes in more general one-dimensional photonic crystals, such as evanescent modes localized in the structure between two semi-infinite one-dimensional photonic crystals. Two photonic crystals can be of same materials, such as shown in Figs. 6 and 10 of Chap. 4 in [12], Figs. 7 and 11 of Chap. 4 in [17], or different materials, such as in Fig. 6 in [30]. The structure in-between can be merely a single interface, a layer of different thickness, or a layer of different material, and so forth.

Besides, we can also obtain some other general understandings of surface modes in one-dimensional photonic crystals from the general mathematical theory.

F.3.3.1 Zeros of the Surface Modes

Theorem 2.8 gives the numbers of zeros of an evanescent mode in each period in a one-dimensional photonic crystal. Based on the theorem, we know that any surface mode in the lowest band gap has exactly one zero in one period, any surface mode in the next lowest band gap has exactly two zeros in one period, such as shown in
Figs. 6.19, 6.20 in [8], Figs. 11.20, 11.21 in [9], Fig. 6 in [38], etc.; any surface mode in the fourth lowest band gap has exactly four zeros in one period, such as shown in Fig. 1 in [37] and Fig. 9 in [38], etc.

**F.3.3.2 How the Frequency of an Existing Surface Mode Depends on the Surface Location \( \tau \)?**

The theory in Appendix D can be used to predict the behaviors of an existing surface mode in a one-dimensional photonic crystal.

According to (D.20), in general, the eigenvalue \( \Lambda = \Omega^2 \) of an existing TM surface mode or an existing TE surface mode satisfies that

\[
\frac{\partial \Lambda}{\partial \tau} = \frac{1}{p(\tau)} [p(\tau) \psi'(\tau)]^2 - [\psi(\tau)]^2 [q(\tau) - \Lambda w(\tau)].
\]

From this equation, by using \( p(x) \), \( q(x) \), and \( w(x) \) obtained from a comparison of Eq. (F.8) or Eq. (F.13) with Eq. (2.2), we obtain that for both an existing TM surface mode or an existing TE surface mode

\[
\frac{\partial \Lambda}{\partial \tau} > 0.
\]

where Eqs. (F.38) and (F.39) for a surface TM mode, or Eqs. (F.52) and (F.53) for a surface TE modes, and \( \epsilon_0 < \epsilon(\tau) \), and that a localized surface mode can only exist if it is below the light line \( \omega < \frac{c}{\sqrt{\epsilon_0}} k_z \) were used.

Equation (F.62) indicates that if a surface TM or TE mode exists in a one-dimensional semi-infinite photonic crystal, the frequency \( \Omega = \Lambda^{1/2} \) of the surface mode always increases as the boundary \( \tau \) goes inside to the photonic crystal. This behavior was observed in previous numerical calculations such as in [38]. The calculated results in Fig. F.1 clearly shows that the frequency of an existing TE surface mode increases as the boundary \( \tau \) goes inside.

\( \Lambda = \Omega^2 \) as a function of \( \tau \) must be a periodic function with a period \( a \). Therefore, if \( \partial \Lambda/\partial \tau > 0 \) in some interval(s) in any specific period, in the same period there must be some other interval(s) where this inequality can not be true. Correspondingly a surface mode—that is, a solution \( \psi(x, \Lambda) \) of Eqs. (F.34) and (F.35) or Eq. (F.38) for a TM mode or a solution \( \psi(x, \Lambda) \) of Eqs. (F.48) and (F.49) or Eq. (F.52) for a TE mode—could not exist in these intervals. There is a statement that “In fact, every periodic material has surface modes for some choice of termination” (p. 61) in [17]. From what we have just understood, a complementary statement that “Every periodic material can have no surface mode in any specific band gap for some choice of termination” is correct as well. Furthermore, for a specific band gap in a specific one-dimensional photonic crystal, very likely there is a way to find out the surface mode existing and non-existing termination intervals.
F.3.3.3 Extra Comments on Surface Modes in Photonic Crystals

Based on what we learned on the surface states and surface bands in electronic crystals, we may make a few extra comments on the surface modes and surface subbands in photonic crystals.

1. A surface mode or surface subband is closely related to a bulk permitted band rather than a band gap in the physics origin. The existence of a surface mode or a surface subband originates from the existence of a bulk permitted band rather than the existence of a band gap. It is only in the one-dimensional cases that a surface mode has to be in a band gap. The “atypical case” in the statement that “In this atypical case, localization does not require a band gap.” (p. 93 in [17]), in fact, is general in higher dimensional cases.

2. Correspondingly, in a multi-dimensional photonic crystal, a surface mode localized most tightly does not have to be in the mid-band-gap, or even in the band-gap at all. The statement that “as a general rule of thumb, we can localize states near the middle of the gap much more tightly than states near the gap’s edge” (p. 53 in [17]) is true only in one-dimensional cases. The “exceptions” in the statement that “There are subtle exceptions to this rule, for example, with certain band structures in two and three dimensions, saddle points in the bands can lead to strong localization away from midgap” (p. 53 in [17]), in fact, can be general in high dimensional cases.

F.4 Modes in One-Dimensional Photonic Crystals of Finite Length

In principle, the mathematical theory presented in Chap. 2 can be used to treat one-dimensional layered photonic crystals of finite length $L = Na$ as well. Nevertheless, due to the continuities of $H_y (E_y)$ and $E_z (H_z)$ for TM (TE) waves at the interfaces between a finite photonic crystal and its external medium, such as vacuum or other dielectric homogeneous medium, in most cases neither $y = 0$ nor $py' = 0$ can be applied at the boundary of a photonic crystal. Consequently similar results—such as that presented for a one-dimensional electronic crystal in Sect. 4.2 or a one-dimensional phononic crystal in Sect. E.3—would not be obtained.

However, there is an impressive work on one-dimensional photonic crystals made of coaxial cables by El Boudouti et al. [51]. There the authors derived theoretically, confirmed by numerical calculations, and then observed experimentally the existence and behavior of two types of modes in finite size one-dimensional coaxial photonic crystals made of $N$ cells with vanishing magnetic field on both ends.

These authors considered structures made of periodic repetitions of a specific type of one-dimensional cells—coaxial cables. They first considered the case where each unit cell is made of two different segments—say, $A$ and $B$—connected in series to each other. Such a unit can be written as $AB$. By using a Green’s function approach, they analytically obtained the dispersion relation of the infinite structure and all eigen
modes of a finite structure containing N unit cells connected in series—here N is a positive integer—with the boundary conditions on both ends of the finite crystal being $H = 0$ (vanishing magnetic field). They obtained $N - 1$ confined modes in each permitted band whose frequencies depend on N and one mode for each band gap whose frequency is determined by the unit cell and does not depend on N. The latter modes are surface modes associated to one of the two surfaces surrounding the structure. These results are similar to that shown in Fig. 4.1 in Chap. 4 for the electronic states in one-dimensional crystals of finite length.

Then they considered cases where the unit cell is composed of an $ABA$ trisegment thus is symmetrical. When connected in series, a finite structure of $N$ unit cells is terminated by a segment $A$ on both ends and is also symmetrical. They again obtained $N - 1$ confined modes in each permitted band and one mode determined by the single unit cell for each band gap, in an investigation of finite size coaxial cable photonic crystals made of $N$ unit cells. Since the unit cell $ABA$ is symmetric, the one mode associated with a band gap is a band edge mode rather than a localized surface mode. These results are similar to that shown in Fig. 4.5 in Chap. 4 for the electronic states in one-dimensional symmetrical crystals of finite length.

These results indicate once more that in simplest cases, a two-end truncation of the one-dimensional periodicity containing $N$ unit cells leads to the consequences summarized in Eq. (8.1).

References

29. A.M. Kosevich, JETP Lett. 74, 559 (2001)
Appendix G
Electronic States in Ideal Cavity Structures

In this Appendix, we investigate the electronic states in cavity structures where a low-dimensional system such as treated in Chaps. 4–7 is removed from an infinite crystal.

For the electronic states in ideal cavity structures treated in this Appendix, we assume that (i) the potential \( v(x) \) or \( v(x) \) outside the cavity is the same as in (4.1) or (5.1) and (ii) the electronic states are completely confined outside the cavity.

G.1 Electronic States in An Ideal Cavity Structure of A One-Dimensional Crystal

An ideal cavity structure of a one-dimensional crystal is a structure formed when a one-dimensional finite crystal bounded at \( \tau \) and \( \tau + L \) was removed from an infinite one-dimensional crystal with a potential period \( a \). Here, \( L = Na \) and \( N \) is a positive integer.

The eigenvalues \( \Lambda \) and eigenfunctions \( \psi(x) \) of the electronic states in such an ideal cavity structure are solutions of the following two equations:

\[
\begin{align*}
-\psi''(x) + [v(x) - \Lambda]\psi(x) &= 0, & x < \tau \text{ or } x > \tau + L, \\
\psi(x) &= 0, & \tau \leq x \leq \tau + L,
\end{align*}
\]

Equation (G.1) can be considered as the equations of electronic states in two separate ideal semi-infinite one-dimensional crystals: one left semi-infinite crystal in the range of \( (-\infty, \tau) \) and one right semi-infinite crystal in the range of \( (\tau + L, +\infty) \). The two ideal semi-infinite crystals are not independent of each other, since \( L = Na \), and \( N \) is a positive integer. For those two semi-infinity crystals, as in Sect. 3.1, we are interested only in the electronic states whose energy depends on the boundary \( \tau \) or \( \tau + L \). The properties and energies of those boundary-dependent electronic states
in the cavity structure can be easily obtained as long as the $\tau$-dependent electronic states in the ideal finite crystal are obtained.

We have presented an analysis of the $\tau$-dependent states in ideal one-dimensional finite crystals in Sect. 4.3. The boundary-dependent electronic states in an ideal cavity structure of a one-dimensional crystal can be easily obtained from that analysis.

We also take a band gap at $k = 0$ as an example. For a specific band gap index $n$, the boundary $\tau$ could be in one of three cases.

1. If $\tau$ is in the set $L(n)$, in the finite crystal bounded at $\tau$ and $\tau + L$, there is an electronic state with a form of $e^{-\beta x} p(x, A)$ $(\beta > 0)$ in the band gap. It is a surface state with an energy $\Lambda$ located near the left boundary $\tau$ of the finite crystal. Correspondingly, $\tau + L$ is also in the set $L(n)$; therefore, there is a surface state with the same form of $e^{-\beta x} p(x, A)$ and energy $\Lambda$ near the left boundary $\tau + L$ of the right semi-infinite crystal $(\tau + L, +\infty)$, whereas no $\tau$-dependent state exists in the left semi-infinite crystal $(-\infty, \tau)$.

2. If $\tau$ is in the set $R(n)$, in the finite crystal bounded at $\tau$ and $\tau + L$, there is an electronic state with a form of $e^{\beta x} p(x, A)$ $(\beta > 0)$ in the band gap. It is a surface state with an energy $\Lambda$ located near the right boundary $\tau + L$ of the finite crystal. Correspondingly, there is a surface state with the same form of $e^{\beta x} p(x, A)$ and energy $\Lambda$ near the right boundary $\tau$ of the left semi-infinite crystal $(-\infty, \tau)$, whereas no $\tau$-dependent state exists in the right semi-infinite crystal $(\tau + L, +\infty)$.

3. If $\tau$ is in the set $M(n)$, a band edge state with a form of $p(x, A)$ and the band edge energy exists in the finite crystal bounded at $\tau$ and $\tau + L$, indicating a confined band edge state periodically distributed in the finite crystal. Correspondingly, a band edge state with the same form of $p(x, A)$ and the same energy $\Lambda$ exists in both the right semi-infinite crystal $(\tau + L, +\infty)$ and the left semi-finite crystal $(-\infty, \tau)$.

Band gaps at $k = \pi/a$ can be similarly analyzed; only a semi-periodic functions $s(x, A)$ should be used instead of the periodic functions $p(x, A)$.

Therefore, the $\tau$-dependent states in such a cavity structure can be obtained similarly to the $\tau$-dependent states in the finite crystal removed.

### G.2 Electronic States in an Ideal Two-Dimensional Cavity Structure of A Three-Dimensional Crystal

A two-dimensional cavity structure in an infinite three-dimensional crystal is a structure formed when a film of a specific orientation and a specific thickness was removed from an infinite crystal. In this section, we are only interested in such cavity structures where an ideal quantum film as investigated in Chap. 5 was removed from an infinite crystal. As in Chap. 5, we assume that the film plane is defined by two primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, $x_3 = \tau_3$ defines the bottom of the removed film and $N_3$ is a positive integer indicating the thickness of the removed film. Such a cavity structure
Each crystal part has two separate parts: an upper semi-infinite crystal part and a lower semi-infinite crystal part.

The electronic states $\hat{\psi}(\hat{k}, x)$ in a two-dimensional cavity are solutions of the following two equations:

\[
\begin{cases}
-\nabla^2 \hat{\psi}(\hat{k}, x) + [v(x) - \hat{\Lambda}] \hat{\psi}(\hat{k}, x) = 0, & x_3 < \tau_3 \text{ or } x_3 > \tau_3 + N_3, \\
\hat{\psi}(\hat{k}, x) = 0, & \tau_3 \leq x_3 \leq \tau_3 + N_3.
\end{cases}
\]  

(G.2)

The electronic states $\hat{\psi}(\hat{k}, x)$ in such a cavity structure are two-dimensional Bloch waves with a wave vector $\hat{k}$ in the film plane.

As in Sect. G.1, we are only interested in the boundary-dependent electronic states in such a cavity structure. These states in such a cavity structure can be similarly obtained as the boundary-dependent states in the removed film treated in Chap. 5: For each bulk energy band $n$ and each wave vector $\hat{k}$ in the film plane, there is one such electronic state in the cavity structure, which can be obtained from (5.11) by assigning a non-divergent $\hat{\phi}_n(\hat{k}, x; \tau_3)$ in the cavity structure:

\[
\hat{\psi}_n(\hat{k}, x; \tau_3) = \begin{cases}
c \hat{\phi}_n(\hat{k}, x; \tau_3), & x_3 < \tau_3 \text{ or } x_3 > \tau_3 + N_3, \\
0, & \tau_3 \leq x_3 \leq \tau_3 + N_3.
\end{cases}
\]  

(G.3)

where $c$ is a normalization constant. Unlike in (5.29), $c$ in (G.3) does not depend on the thickness $N_3$ of the removed film. The divergent part of $\hat{\phi}_n(\hat{k}, x; \tau_3)$ in (G.3) should be abandoned. Correspondingly, the energy of such a state is given by

\[
\hat{\Lambda}_n(\hat{k}; \tau_3) = \hat{\lambda}_n(\hat{k}; \tau_3),
\]  

(G.4)

as in (5.30). There is one solution (G.3) of (G.2) for each energy band $n$ and each $\hat{k}$. Each $\hat{\psi}_n(\hat{k}, x; \tau_3)$ defined in (G.3) is an electronic state in the cavity structure whose energy $\hat{\Lambda}_n(\hat{k}; \tau_3)$ in (G.4) depends on the cavity boundary $\tau_3$ but not on the cavity size $N_3$. By Theorem 5.1, $\hat{\Lambda}_n(\hat{k}; \tau_3)$ is either above or at the energy maximum of $\varepsilon_n(k)$ with that $n$ and that $\hat{k}$.

In the special cases where $\hat{\phi}_n(\hat{k}, x; \tau_3)$ in (G.3) is a Bloch function,

\[
\hat{\phi}_n(\hat{k}, x; \tau_3) = \phi_n(k, x), \quad n \leq n',
\]  

(G.5)

the corresponding Bloch function $\phi_{n'}(k, x)$ has a nodal surface at $x_3 = \tau_3$ and thus has nodal surfaces at $x_3 = \tau_3 + \ell$, where $\ell = 1, 2, \ldots, N_3$. The wave function $\hat{\phi}_n(\hat{k}, x; \tau_3)$ in (G.3) exists in both the upper semi-infinite crystal part and the lower semi-infinite crystal part of the cavity structure.

In most cases, $\hat{\phi}_n(\hat{k}, x; \tau_3)$ in (G.3) is not a Bloch function. In such a situation there is a nonzero imaginary part of $k_3$ in (5.11), indicating that $\hat{\psi}_n(\hat{k}, x; \tau_3)$ in (G.3) is a surface state located near either the top surface of the lower semi-infinite crystal part (if the imaginary part of $k_3$ in (5.11) is negative) or the bottom surface of the
upper semi-infinite crystal part (if the imaginary part of $k_3$ in (5.11) is positive) of the cavity structure: It exists in one of the two semi-infinite crystal parts of the cavity structure: for some $\mathbf{k}$ it is in the upper part above the cavity, whereas for some other $\mathbf{\hat{k}}$ it is in the lower part below the cavity. Correspondingly, the energy of such a state

\[ \hat{\Lambda}_n(\mathbf{\hat{k}}; \tau_3) > \epsilon_n(\mathbf{k}), \quad \text{for } (\mathbf{k} - \mathbf{\hat{k}}) \cdot \mathbf{a}_i = 0, \quad i = 1, 2, \]  

(G.6)

by Theorem 5.1. However, there is no reason to expect that $\hat{\Lambda}_n(\mathbf{\hat{k}}; \tau_3)$ has to be in a band gap.

Therefore, for each bulk energy band $n$, there is one surface-like subband $\hat{\Lambda}_n(\mathbf{\hat{k}}; \tau_3)$ in (G.4) in such an ideal cavity structure.

Those results should be correct for cavity structures of crystals with a sc, tetr, or an ortho Bravais lattice for which an ideal (001) film was removed. More generally, they should also be correct for ideal cavity structures of crystals with an fcc or a bcc Bravais lattice for which an ideal (001) or (110) film was removed.

We have seen in Sects. G.1 and G.2 that the boundary-dependent electronic states in a cavity structure actually can be obtained similarly to the boundary-dependent electronic states in the removed low-dimensional systems. This is due to the mere fact that the ideal cavity structure and the ideal low-dimensional system removed have the same boundary. The same idea can be applied to obtain the boundary-dependent electronic states in an ideal one-dimensional or zero-dimensional cavity structure in a three-dimensional crystal.

G.3 Electronic States in an Ideal One-Dimensional Cavity Structure of a Three-Dimensional Crystal

A one-dimensional cavity structure in a three-dimensional crystal is a structure formed when a quantum wire was removed from an infinite crystal. In this section, we are only interested in such cavity structures where an ideal rectangular quantum wire investigated in Chap. 6 was removed from an infinite crystal.

As in Chap. 6, we choose the primitive vector $\mathbf{a}_1$ in the wire cavity direction. Such a rectangular wire cavity can be defined by a bottom face $x_3 = \tau_3$, a top face $x_3 = \tau_3 + N_3$, a front face perpendicularly intersecting the $\mathbf{a}_2$ axis at $\tau_2 \mathbf{a}_2$, and a rear face perpendicularly intersecting it at $(\tau_2 + N_2) \mathbf{a}_2$. Here, $\tau_2$ and $\tau_3$ define the boundary faces of the wire cavity, and $N_2$ and $N_3$ are two positive integers indicating the size and shape of the wire cavity.

For the electronic states in such an ideal cavity structure, we look for the eigenvalues $\Lambda$ and eigenfunctions $\hat{\psi}(\mathbf{k}, \mathbf{x})$ of the following two equations:

\[
\begin{cases}
-\nabla^2 \hat{\psi}(\mathbf{k}, \mathbf{x}) + [v(\mathbf{x}) - \Lambda] \hat{\psi}(\mathbf{k}, \mathbf{x}) = 0, & \mathbf{x} \notin \text{the cavity}, \\
\hat{\psi}(\mathbf{k}, \mathbf{x}) = 0, & \mathbf{x} \in \text{the cavity}.
\end{cases}
\]  

(G.7)

The solutions $\hat{\psi}(\mathbf{k}, \mathbf{x})$ of (G.7) are one-dimensional Bloch waves with a wave vector $\mathbf{\hat{k}}$ in the wire direction $\mathbf{a}_1$. 
There are different types of electronic state solutions of these two equations. As in Sects. G.1 and G.2, in this section, we are only interested in the solutions of (G.7) whose energies are dependent on the cavity boundary locations \( \tau_2 \) and/or \( \tau_3 \). Based on similar arguments we had in Chaps. 5–6 and in Sects. G.1 and G.2, we can understand that the electronic states whose energies are dependent on the cavity boundary location \( \tau_2 \) or \( \tau_3 \) are surface-like states in the cavity structure. They are located near the opposite surface of the cavity structure in comparison with the corresponding surface-like states in the removed quantum wire: If there is a surface-like state located near the top surface of the removed quantum wire, then there is a corresponding surface-like state located near the bottom surface of the cavity and vice versa. If there is a surface-like state located near the front surface of the removed quantum wire, then there is a corresponding surface-like state located near the rear surface of the cavity and vice versa. Similarly, the electronic states whose energies are dependent on the cavity boundary locations \( \tau_2 \) and \( \tau_3 \) are edge-like states in the cavity structure; they are located near the opposite edge of the cavity in comparison with the corresponding edge-like states in the removed quantum wire.

**G.3.1 Wire Cavities in Crystals with A sc, tetr, or ortho Bravais Lattice**

For an ideal one-dimensional cavity structure of a crystal with a sc, tetr, or ortho Bravais lattice, we consider the case where the rectangular quantum wire removed has two boundary faces at \( x_3 = \tau_3 \) and \( x_3 = \tau_3 + N_3 \) in the \( a_3 \) direction, two other boundary faces at \( x_2 = \tau_2 \) and \( x_2 = \tau_2 + N_2 \) in the \( a_2 \) direction. For each bulk energy band \( n \) in the cavity structure, there are

\[
\bar{\Lambda}_{n,j_3}(\vec{k}; \tau_2) = \hat{\Lambda}_n(\vec{k} + \frac{j_3 \pi}{N_3} \hat{b}_3; \tau_2);
\]

(G.8)

\((N_3 - 1)\) surface-like subbands with energies

\[
\bar{\Lambda}_{n,j_2}(\vec{k}; \tau_3) = \hat{\Lambda}_n(\vec{k} + \frac{j_2 \pi}{N_2} \hat{b}_2; \tau_3);
\]

(G.9)

\((N_2 - 1)\) surface-like subbands with energies

one edge-like subband with energy \( \bar{\Lambda}_n(\vec{k}; \tau_2, \tau_3) \) depending on both \( \tau_2 \) and \( \tau_3 \), similar to (6.29), (6.30), and (6.31) in Sect. 6.4.

Here, \( j_2 = 1, 2, \ldots, N_2 - 1 \) and \( j_3 = 1, 2, \ldots, N_3 - 1 \). \( \hat{\Lambda}_n(\vec{k}; \tau_3) \) is the surface-like band structure in a quantum film with the film plane oriented in the \( a_3 \) direction. \( \hat{\Lambda}_n(\vec{k}; \tau_2) \) is the surface-like band structure in a quantum film with the film plane oriented in the \( a_2 \) direction.
However, probably the practically more interesting cases are cavity structures of crystals with an fcc or bcc Bravais lattice. In the following, we give predictions on the electronic states in several such one-dimensional cavity structures.

G.3.2 Wire Cavities with (001) and (110) Surfaces in an fcc Crystal

A cavity structure with (001) and (110) surfaces in an fcc crystal is a structure formed when an [1\bar{1}0] quantum wire was removed from an infinite crystal with an fcc Bravais lattice. The removed quantum wire has (001) and (110) surfaces and has a rectangular cross section \( N_{110}a/\sqrt{2} \times N_{001}a \), where \( N_{110} \) and \( N_{001} \) are two positive integers.

For each bulk energy band \( n \), there are \( (N_{001} - 1) + (N_{110} - 1) \) surface-like subbands in such a cavity structure. They are \((N_{001} - 1)\) subbands with energies

\[
\bar{\Lambda}_{sf,1}^{n,j_{001}}(\vec{k}; \tau_{110}) = \hat{\Lambda}_n \left[ \vec{k} + \frac{j_{001}\pi}{N_{001}a} (0, 0, 1); \tau_{110} \right] \quad \text{(G.10)}
\]

and \((N_{110} - 1)\) subbands with energies

\[
\bar{\Lambda}_{sf,2}^{n,j_{110}}(\vec{k}; \tau_{001}) = \hat{\Lambda}_n \left[ \vec{k} + \frac{j_{110}\pi}{N_{110}a} (1, 1, 0); \tau_{001} \right] \quad \text{(G.11)}
\]

similar to (6.51) and (6.52). Here, \( \tau_{001} \) or \( \tau_{110} \) define the boundary faces of the cavity in the [001] or [110] direction, \( j_{001} = 1, 2, \ldots, N_{001} - 1 \), and \( j_{110} = 1, 2, \ldots, N_{110} - 1 \).

\( \hat{\Lambda}_n(\vec{k}; \tau_{001}) \) is the surface-like band structure in a quantum film with the film plane oriented in the [001] direction. \( \hat{\Lambda}_n(\vec{k}; \tau_{110}) \) is the surface-like band structure in a quantum film with the film plane oriented in the [110] direction.

For each bulk energy band \( n \), there is one edge-like subband in the cavity structure with energy \( \bar{\Lambda}_{eg}^{n}(\vec{k}; \tau_{001}, \tau_{110}) \) depending on both \( \tau_{001} \) and \( \tau_{110} \), similar to (6.38) or (6.45).

G.3.3 Wire Cavities with (110) and (1\bar{1}0) Surfaces in an fcc Crystal

A cavity structure with (110) and (1\bar{1}0) surfaces in an fcc crystal is a structure formed when a [001] quantum wire was removed from an infinite crystal with an fcc Bravais lattice. The removed quantum wire has (110) and (1\bar{1}0) surfaces and has a rectangular cross section \( N_{110}a/\sqrt{2} \times N_{1\bar{1}0}a/\sqrt{2} \), where \( N_{110} \) and \( N_{1\bar{1}0} \) are two positive integers.

For each bulk energy band \( n \), there are \( (N_{1\bar{1}0} - 1) + (N_{110} - 1) \) surface-like subbands in the cavity structure. They are \((N_{1\bar{1}0} - 1)\) subbands with energies
\[
\bar{\Lambda}_{n,j_{110}}^{sf,a_1}(\mathbf{k}; \tau_{110}) = \hat{\Lambda}_n \left[ \mathbf{k} + \frac{j_{110}\pi}{N_{110}a} (1, -1, 0); \tau_{110} \right] \quad (G.12)
\]

and \((N_{110} - 1)\) subbands with energies

\[
\bar{\Lambda}_{n,j_{110}}^{sf,a_2}(\mathbf{k}; \tau_{110}) = \hat{\Lambda}_n \left[ \mathbf{k} + \frac{j_{110}\pi}{N_{110}a} (1, 1, 0); \tau_{110} \right], \quad (G.13)
\]

similar to \((6.61)\) and \((6.62)\). Here, \(\tau_{110}\) or \(\tau_{110}\) define the boundary faces of the cavity in the [110] or [\(\bar{1}10\)] direction, \(j_{110} = 1, 2, \ldots, N_{110} - 1\), and \(j_{110} = 1, 2, \ldots, N_{110} - 1\).

\(\hat{\Lambda}_n(\mathbf{k}; \tau_{110})\) is the surface-like band structure in a quantum film with the film plane oriented in the [110] direction. \(\hat{\Lambda}_n(\mathbf{k}; \tau_{110})\) is the surface-like band structure in a quantum film with the film plane oriented in the [110] direction.

For each bulk energy band \(n\), there is one edge-like subband in the cavity structure with energy \(\bar{\Lambda}_{n}^{eg}(\mathbf{k}; \tau_{110}, \tau_{110})\) depending on both \(\tau_{110}\) and \(\tau_{110}\), similar to \((6.63)\).

### G.3.4 Wire Cavities with (010) and (001) Surfaces in a bcc Crystal

A cavity structure with (010) and (001) surfaces in a bcc crystal is a structure formed when a [100] quantum wire was removed from an infinite crystal with a bcc Bravais lattice. The removed quantum wire has (010) and (001) surfaces and has a rectangular cross section \(N_{010}a \times N_{001}a\), where \(N_{010}\) and \(N_{001}\) are two positive integers.

For each bulk energy band \(n\), there are \((N_{001} - 1) + (N_{010} - 1)\) surface-like subbands in the cavity structure. They are \((N_{001} - 1)\) subbands with energies

\[
\bar{\Lambda}_{n,j_{001}}^{sf,a_1}(\mathbf{k}; \tau_{010}) = \hat{\Lambda}_n \left[ \mathbf{k} + \frac{j_{001}\pi}{N_{001}a} (0, 0, 1); \tau_{010} \right] \quad (G.14)
\]

and \((N_{010} - 1)\) subbands with energies

\[
\bar{\Lambda}_{n,j_{001}}^{sf,a_2}(\mathbf{k}; \tau_{001}) = \hat{\Lambda}_n \left[ \mathbf{k} + \frac{j_{010}\pi}{N_{010}a} (0, 1, 0); \tau_{001} \right], \quad (G.15)
\]

similar to \((6.69)\) and \((6.70)\). Here, \(\tau_{010}\) or \(\tau_{001}\) define the boundary faces of the cavity in the [010] or [001] direction, \(j_{001} = 1, 2, \ldots, N_{001} - 1\), and \(j_{010} = 1, 2, \ldots, N_{010} - 1\).

\(\hat{\Lambda}_n(\mathbf{k}; \tau_{001})\) is the surface-like band structure in a quantum film with the film plane oriented in the [001] direction. \(\hat{\Lambda}_n(\mathbf{k}; \tau_{010})\) is the surface-like band structure in a quantum film with the film plane oriented in the [010] direction.

For each bulk energy band \(n\), there is one edge-like subband in the cavity structure with energy \(\bar{\Lambda}_{n}^{eg}(\mathbf{k}; \tau_{001}, \tau_{010})\) depending on both \(\tau_{001}\) and \(\tau_{010}\), similar to \((6.71)\).
G.4 Electronic States in an Ideal Zero-Dimensional Cavity Structure of a Three-Dimensional Crystal

A zero-dimensional cavity structure in an infinite three-dimensional crystal is a structure formed when a quantum dot was removed from the infinite crystal. In this section, we are only interested in ideal cavity structures where a quantum dot of rectangular cuboid shape investigated in Chap. 7 was removed from an infinite crystal.

Such a cavity can be defined by a bottom and top face at \( x_3 = \tau_3 \) and \( x_3 = \tau_3 + N_3 \), a front and rear face perpendicularly intersecting the \( a_2 \) axis at \( x_2 = \tau_2 \) and \( x_2 = \tau_2 + N_2 \), and a left and right face perpendicularly intersecting the \( a_1 \) axis at \( x_1 = \tau_1 \) and \( x_1 = \tau_1 + N_1 \). Here, \( \tau_1, \tau_2, \) and \( \tau_3 \) define the boundary faces of the cavity and \( N_1, N_2, \) and \( N_3 \) are three positive integers indicating the cavity size and/or shape. We look for the eigenvalues \( \Lambda \) and eigenfunctions \( \psi(x) \) of the following two equations:

\[
\begin{cases}
-\nabla^2 \psi(x) + [v(x) - \Lambda] \psi(x) = 0, & x \notin \text{the cavity}, \\
\psi(x) = 0, & x \in \text{the cavity}.
\end{cases}
\]  

(G.16)

There are different types of electronic state solutions of (G.16). As in Sects. G.1–G.3, in this section, we are only interested in the solutions of (G.16) whose energies are dependent on the cavity boundary \( \tau_1, \tau_2, \) and/or \( \tau_3 \). Based on similar arguments we had in Chaps. 5–7 and in Sects. G.1–G.3, we can understand that the electronic states whose energies are dependent on one of the cavity boundary locations \( \tau_1, \tau_2, \) or \( \tau_3 \) are surface-like states in the cavity structure; they are located near the opposite surface of the cavity structure in comparison with the corresponding surface-like states in the removed quantum dot: If there is a surface-like state located near one specific surface in the removed quantum dot, then there is a corresponding surface-like state located near the opposite surface of the cavity. The electronic states whose energies are dependent on two of the cavity boundary locations \( \tau_1, \tau_2, \) or \( \tau_3 \) are edge-like states in the cavity structure; they are located near the opposite edge of the cavity in comparison with the corresponding edge-like states in the removed quantum dot. The electronic states whose energies are dependent on all three cavity boundary locations \( \tau_1, \tau_2, \) and \( \tau_3 \) are vertex-like states in the cavity structure; they are located near the opposite vertex of the cavity in comparison with the corresponding vertex-like states in the removed quantum dot.

G.4.1 Dot Cavities In Crystals with a sc, tetr, or ortho Bravais Lattice

For such a cavity structure with sizes \( N_1a_1, N_2a_2 \) and \( N_3a_3 \) in the \( a_1, a_2 \) and \( a_3 \) directions in a crystal with a sc, tetr, or ortho Bravais lattice, for each bulk energy band there are \((N_1 - 1)(N_2 - 1) + (N_2 - 1)(N_3 - 1) + (N_3 - 1)(N_1 - 1)\) surface-like states, \((N_1 - 1) + (N_2 - 1) + (N_3 - 1)\) edge-like states, and one vertex-like state in the cavity structure. They are as follows:
$(N_1 - 1)(N_2 - 1)$ surface-like states with energies

$$\Lambda_{n, j_1, j_2}(\tau_3) = \hat{\Lambda}_n \left[ \frac{j_1\pi}{N_1} b_1 + \frac{j_2\pi}{N_2} b_2; \tau_3 \right]; \quad (G.17)$$

$(N_2 - 1)(N_3 - 1)$ surface-like states with energies

$$\Lambda_{n, j_2, j_3}(\tau_1) = \hat{\Lambda}_n \left[ \frac{j_2\pi}{N_2} b_2 + \frac{j_3\pi}{N_3} b_3; \tau_1 \right]; \quad (G.18)$$

$(N_3 - 1)(N_1 - 1)$ surface-like states with energies

$$\Lambda_{n, j_3, j_1}(\tau_2) = \hat{\Lambda}_n \left[ \frac{j_3\pi}{N_3} b_3 + \frac{j_1\pi}{N_1} b_1; \tau_2 \right]; \quad (G.19)$$

$(N_1 - 1)$ edge-like states with energies

$$\Lambda_{n, j_1}(\tau_2, \tau_3) = \Lambda_n \left[ \frac{j_1\pi}{N_1} b_1; \tau_2, \tau_3 \right]; \quad (G.20)$$

$(N_2 - 1)$ edge-like states with energies

$$\Lambda_{n, j_2}(\tau_3, \tau_1) = \Lambda_n \left[ \frac{j_2\pi}{N_2} b_2; \tau_3, \tau_1 \right]; \quad (G.21)$$

$(N_3 - 1)$ edge-states with energies

$$\Lambda_{n, j_3}(\tau_1, \tau_2) = \Lambda_n \left[ \frac{j_3\pi}{N_3} b_3; \tau_1, \tau_2 \right]; \quad (G.22)$$

and one vertex-like state with energy $\Lambda_n(\tau_1, \tau_2, \tau_3)$ depending all three $\tau_1$, $\tau_2$, and $\tau_3$, similar to (7.39)–(7.45).

Here $j_1 = 1, 2, \ldots, N_1 - 1$, $j_2 = 1, 2, \ldots, N_2 - 1$, and $j_3 = 1, 2, \ldots, N_3 - 1$. $\tau_1$, $\tau_2$, and $\tau_3$ define the boundary faces of the cavity in the $a_1$, $a_2$, and $a_3$ directions. $\hat{\Lambda}_n[k; \tau_l]$ is the surface-like band structure of a quantum film with the film plane oriented in the $a_l$ direction. $\Lambda_n[k; \tau_l, \tau_m]$ is the edge-like band structure of a rectangular quantum wire with the wire faces oriented in the $a_l$ or the $a_m$ direction.

Probably the practically more interesting cases are the cavity structures in crystals with an fcc or bcc Bravais lattice. Similar to Sects. G.1–G.3, electronic states in those cavity structures can be obtained.
G.4.2 Dot Cavities with (\(\bar{1}10\)), (110), and (001) Surfaces in An fcc Crystal

For a cavity structure in a crystal with an fcc Bravais lattice, if the cavity has (001), (110), and (\(\bar{1}10\)) surfaces and a rectangular cuboid size \(N_{001}a \times N_{110}a / \sqrt{2} \times N_{\bar{1}10}a / \sqrt{2}\), the boundary-dependent electronic states in such a cavity structure can be obtained similarly to the boundary-dependent electronic states in an ideal quantum dot obtained in Sect. 7.7.

For each bulk energy band \(n\), there are \((N_{001} - 1)(N_{\bar{1}10} - 1) + (N_{110} - 1)(N_{001} - 1) + (N_{\bar{1}10} - 1)(N_{110} - 1)\) surface-like states in the cavity structure. They are as follows:

\[ (N_{001} - 1)(N_{\bar{1}10} - 1) \] states with energies

\[
A_{n, j_{001} = 1}^{sf, a_{01}} (\tau_{110}) = \tilde{A}_n \left[ \frac{j_{001} \pi}{N_{001}a} (0, 0, 1) + \frac{j_{110} \pi}{N_{110}a} (1, -1, 0); \tau_{110} \right],
\] (G.23)

\[(N_{110} - 1)(N_{001} - 1) \] states with energies

\[
A_{n, j_{110} = 1}^{sf, a_{02}} (\tau_{110}) = \tilde{A}_n \left[ \frac{j_{110} \pi}{N_{110}a} (0, 0, 1) + \frac{j_{001} \pi}{N_{001}a} (1, -1, 0); \tau_{110} \right],
\] (G.24)

\[(N_{\bar{1}10} - 1)(N_{110} - 1) \] states with energies

\[
A_{n, j_{\bar{1}10} = 1}^{sf, a_{03}} (\tau_{001}) = \tilde{A}_n \left[ \frac{j_{\bar{1}10} \pi}{N_{\bar{1}10}a} (1, -1, 0) + \frac{j_{110} \pi}{N_{110}a} (1, 1, 0); \tau_{001} \right],
\] (G.25)

similar to (7.56)–(7.58).

Here, \(j_{001} = 1, 2, \ldots, N_{001} - 1\), \(j_{110} = 1, 2, \ldots, N_{110} - 1\), and \(j_{\bar{1}10} = 1, 2, \ldots, N_{\bar{1}10} - 1\). \(\tau_{110}, \tau_{\bar{1}10}, \) or \(\tau_{001}\) define the boundary faces of the cavity in the [110], [\(\bar{1}10\)], or [001] direction. \(\tilde{A}_n [\tilde{k}; \tau]\) is the surface-like band structure of a quantum film with the film plane oriented in the [\(l\)] direction. \(l\) can be either one of 110, \(\bar{1}10\), or 001.

For each energy band \(n\), there are \((N_{001} - 1) + (N_{110} - 1) + (N_{\bar{1}10} - 1)\) edge-like states in the cavity structure. They are as follows:

\[(N_{001} - 1) \] states with energies

\[
A_{n, j_{001} = 1}^{eg, a_{01}} (\tau_{110}, \tau_{\bar{1}10}) = \tilde{A}_n \left[ \frac{j_{001} \pi}{N_{001}a} (0, 0, 1); \tau_{110}, \tau_{\bar{1}10} \right],
\] (G.26)

\[(N_{110} - 1) \] states with energies

\[
A_{n, j_{110} = 1}^{eg, a_{02}} (\tau_{110}, \tau_{001}) = \tilde{A}_n \left[ \frac{j_{110} \pi}{N_{110}a} (1, 1, 0); \tau_{110}, \tau_{001} \right],
\] (G.27)
Appendix G: Electronic States in Ideal Cavity Structures

\((N_{110} - 1)\) states with energies

\[
\Lambda_{n,j_{110}}^{eg,as}(\tau_{001}, \tau_{110}) = \tilde{A}_n \left[ \frac{j_{110}\pi}{N_{110}a} (1, -1, 0); \tau_{001}, \tau_{110} \right].
\]

(G.28)

similar to (7.59)–(7.61).

Here, \(\tilde{A}_n[\tilde{k}; \tau_l, \tau_m]\) is the edge-like band structure of a rectangular quantum wire with the wire faces oriented in the \([l]\) or the \([m]\) direction. \(l\) and \(m\) can be two of 001, 110, and \(\bar{1}10\).

For each bulk energy band \(n\), there is one vertex-like state in the cavity structure with energy \(\Lambda_{vt}^n(\tau_{001}, \tau_{110}, \tau_{100})\) depending all three \(\tau_{001}, \tau_{110},\) and \(\tau_{100}\), similar to (7.62).

\[\]

\[\]

\[\]

\[\]

G.4.3 Dot Cavities with (100), (010), and (001) Surfaces in bcc Crystals

In a crystal with a bcc Bravais lattice, the boundary-dependent electronic states in a cavity structure with (100), (010) and (001) surfaces and a rectangular cuboid size \(N_{100}a \times N_{010}a \times N_{001}a\) can be obtained similarly to the boundary-dependent electronic states in an ideal quantum dot obtained in Sect. 7.8.

For each bulk energy band \(n\), there are \((N_{100} - 1)(N_{010} - 1)\) states with energies \(\Lambda_{n,j_{010},j_{001}}^{sf,as}(\tau_{100})\) depending all three \(\tau_{001}, \tau_{110},\) and \(\tau_{100}\), similar to (7.72)–(7.74).

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similar to (7.72)–(7.74).

Here, \(j_{100} = 1, 2, \ldots, N_{100} - 1, j_{010} = 1, 2, \ldots, N_{010} - 1, \) and \(j_{001} = 1, 2, \ldots, N_{001} - 1. \) \(\tau_{100}, \tau_{010}, \) or \(\tau_{001}\) define the boundary faces of the cavity in the \([100], [010],\) or \([001]\) direction. \(\tilde{A}_n[\tilde{k}; \tau_l]\) is the surface-like band structure of a
quantum film with the film plane oriented in the \([l]\) direction. \(l\) can be either one of 100, 010, or 001.

For each bulk energy band \(n\), there are \((N_{100} - 1) + (N_{010} - 1) + (N_{001} - 1)\) edge-like states in the cavity structure. They are as follows:

\((N_{100} - 1)\) states with energies

\[
\Lambda_{n,j_{100}}^{eg, a_1} (\tau_{010}, \tau_{001}) = \bar{A}_n \left[ j_{100} \frac{\pi}{N_{100} a} (1, 0, 0); \tau_{010}, \tau_{001} \right]; \tag{G.32}
\]

\((N_{010} - 1)\) states with energies

\[
\Lambda_{n,j_{010}}^{eg, a_2} (\tau_{001}, \tau_{100}) = \bar{A}_n \left[ j_{010} \frac{\pi}{N_{010} a} (0, 1, 0); \tau_{001}, \tau_{100} \right]; \tag{G.33}
\]

\((N_{001} - 1)\) states with energies

\[
\Lambda_{n,j_{001}}^{eg, a_3} (\tau_{100}, \tau_{010}) = \bar{A}_n \left[ j_{001} \frac{\pi}{N_{001} a} (0, 0, 1); \tau_{100}, \tau_{010} \right], \tag{G.34}
\]

similar to \((7.75)–(7.77)\).

Here, \(\bar{A}_n[k; \tau_l, \tau_m]\) is the edge-like band structure of a rectangular quantum wire with the wire faces oriented in the \([l]\) or the \([m]\) direction. \(l\) and \(m\) can be two of 100, 010, and 001.

For each bulk energy band \(n\), there is one vertex-like state in the cavity structure with energy \(\Lambda_{n}^{vt} (\tau_{100}, \tau_{010}, \tau_{001})\) depending all three \(\tau_{100}, \tau_{010},\) and \(\tau_{001}\), similar to \((7.78)\).
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