Tangent formulation of the Kronig-Penney problem for *N*-period layered systems with application to photonic crystals

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At symmetry points of the Brillouin zone, the two-layer Kronig-Penney (KP) problem has even- and odd-parity solutions that are expressible with tangents and cotangents. Similar solutions are derived here for an arbitrary number of layers. Namely, the eigenvalue-eigenvector problem for the energy spectra and wave functions of arbitrary, one-dimensional, ***N***-period layered systems is formulated in terms of tangents only. The resulting equations are compact, algorithmically simple, numerically stable, and physically appealing. The derived secular equation is Hermitian and only of order $N\times N$ (i.e., half the size of the KP secular equation). The eigenfrequency condition has physically attractive geometric representation in terms of N-sided figures such as triangles and tetrahedrons for $N=3$. The analytic power of the formalism is demonstrated by diagonalizing the secular equation for $N=3$, finding a factored form of the KP equation, and deriving analytic eigenfrequency conditions and analytic wave functions for the three layer problem. The analyticity of the formalism should aid the band-gap engineering of the band structure and wave functions of multilayer structures. The numerical ease of implementation is demonstrated by calculating the eigenfrequencies and wave functions for a three-layer photonic crystal.

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I. INTRODUCTION

One-dimensional periodic systems with N layers per period pervade many areas of physics.[1–9] The eigenvalue conditions for such systems are given by the simple and elegant Kronig-Penney (KP) equation.[10] For $N=2$, the KP problem has separate even- and odd-parity solutions in the form of tangents and cotangents.[11] However, for $N>2$, the KP equation becomes algorithmically complicated and its tangent form is unknown. The overall eigenvector-eigenvalue problem is represented by a complex, non-Hermitian, $2N\times 2N$ equation. Alternatively, the problem can be solved in the transfer matrix formalism,[12] which involves a multiplication of N, 2×2 complex, non-Hermitian transfer matrices.

This paper derives the tangent form for a N-layer periodic problem and explores its physical and mathematical consequences. For ease of reading, Appendix A contains the glossary of terms and notation used in this paper. The eigenvalue condition for an arbitrary, one-dimensional periodic system with N layers per period is constructed from the boundary conditions for the N forward- and N backward-propagating wave amplitudes, Sec. II. A generalized KP model is set up in Sec. III using the compact notation developed in Sec. II. For later comparison, a three-layer photonic band-gap material (PBG) is used as an example of the standard KP approach. An alternative formulation of the problem in terms of tangents is presented in Sec. IV, where it is shown to assume the form of a Hermitian $2N\times 2N$ eigenvalue-eigenvector problem and is written compactly as a 2×2 matrix comprising four $N\times N$ block matrices—thenceforth called the main equation. The resulting expression has the form of the operator Riccati equation.[13–17] Since this paper demonstrates the results for N odd, Appendix B shows how to derive the corresponding formulas for N even. For the purposes of this paper, N-even results are found using the N-odd formalism in the limit of one of the layer widths approaching zero. Using the example of the three-layer PBG, the resulting formalism is shown to be numerically equivalent to the standard KP formulation of Sec. II.

Next, in Secs. V and VI, the main equation is block diagonalized and reduced to a $N\times N$ Hermitian form—called the submain equation—that is half the size of the corresponding KP formalism. At symmetry points, the submain equation is real, which makes it possible to interpret the eigenfrequency condition in terms of geometric figures—for example, triangles and/or tetrahedrons for $N=3$; for general N, the eigenvalue condition can be represented in terms of N-sided figures in $(N-1)$-dimensional space. The use of the submain equation is shown to be equivalent to the use of the main equation itself. Using the example of $N=3$, Sec. VII diagonalizes the submain equation and derives analytic eigenfrequency conditions and wave functions. Conclusions are given last.

II. FORMALISM DEVELOPMENT AND NOTATION

Consider a periodic structure with N layers per period, where the ith layer extends between $z_{i-1}\leqslant z\leqslant z_i$, its width is $z_i-z_{i-1}=2a_i$, for $1\leqslant i\leqslant N$, and $z_0\equiv 0$. The period $d=2(a_1+a_2+a_3+\cdots+a_N)$. In what follows, matrices will be denoted in boldface capitals.

Without a loss of generality, this development is applied to PBG's, a periodic system of dielectric layers, in which the propagation of a plane electromagnetic wave in the z direction is governed by the wave equation[18,19]

$$\left[\frac{d^2}{dz^2}+k^2(z)\right]\psi(z)=0, \tag{1}$$

where $\psi(z)$ refers to Cartesian components of the electric or magnetic field, the propagation wave vector $k_i=2\pi n_i/\lambda$, n_i is the refractive index, and λ is the wavelength in vacuum.[20] The photonic bands $\lambda(q)$ are periodic functions of q, where the wave vector $-\pi/d < q \leq \pi/d$, with the period $2\pi/d$. Moreover, the solutions must obey the Bloch periodicity condition[10,11]

$$\psi(z+d) = \exp(iqd)\psi(z). \tag{2}$$

In the ith layer of the zeroth period, the solution is a superposition of right/left (+/−) traveling waves

$$\psi(z) = c_i^+ \exp(ik_i z) + c_i^- \exp(-ik_i z), \quad z_{i-1} \leq z \leq z_i. \tag{3}$$

The wave amplitudes ψ and their derivatives $d\psi/dz$ (TE mode) and $n^{-2}d\psi/dz$ (TM mode) are continuous at all interfaces.[20] For economy of notation and transparency, common quantities are grouped together as[21]

$$\boldsymbol{M}_i = \begin{pmatrix} 1 & 1 \\ \alpha_i & -\alpha_i \end{pmatrix}, \tag{4}$$

where $\alpha_i = (n_i, n_i^{-1})$ for (TE/TM) modes, so that $\boldsymbol{M}$ contains materials information only.[22,23] The 2×1 eigenvector for the ith layer,

$$\boldsymbol{C}_i = \begin{pmatrix} c_i^+ \\ c_i^- \end{pmatrix}, \tag{5}$$

and the diagonal matrix for the propagation wave vectors,

$$\boldsymbol{K}_i = \begin{pmatrix} k_i & 0 \\ 0 & -k_i \end{pmatrix}. \tag{6}$$

Using Eq. (6), it follows that the matrix exponential

$$\exp(i\boldsymbol{K}_i a_i) = \begin{pmatrix} \exp(ik_i a_i) & 0 \\ 0 & \exp(-ik_i a_i) \end{pmatrix}, \tag{7}$$

which is diagonal and contains all the dimensional (structural) information. In this notation both boundary conditions at $z=z_i$ are expressed as[22,23]

$$\boldsymbol{M}_i \exp(i\boldsymbol{K}_i z_i)\boldsymbol{C}_i = \boldsymbol{M}_{i+1} \exp(i\boldsymbol{K}_{i+1} z_i)\boldsymbol{C}_{i+1}, \quad i = 1, \ldots, N-1; \tag{8}$$

for the last layer $i=N$, the boundary condition supplemented by the Bloch periodicity condition yields

$$\boldsymbol{M}_N \exp(i\boldsymbol{K}_N z_N)\boldsymbol{C}_N = \exp(iqd)\boldsymbol{M}_1 \exp(i\boldsymbol{K}_1 z_0)\boldsymbol{C}_1. \tag{9}$$

One can use Eqs. (4)–(7) to define another matrix exponential

$$\exp(i\boldsymbol{\Lambda}_i z_i) \equiv \boldsymbol{M}_i \exp(i\boldsymbol{K}_i z_i)\boldsymbol{M}_i^{-1} = \begin{pmatrix} \cos k_i z_i & i \sin k_i z_i/\alpha_i \\ i\alpha_i \sin k_i z_i & \cos k_i z_i \end{pmatrix} \tag{10}$$

and the matrix tangent

$$\tan \boldsymbol{\Lambda}_i z_i \equiv \boldsymbol{M}_i \tan(\boldsymbol{K}_i z_i)\boldsymbol{M}_i^{-1} = \begin{pmatrix} 0 & \tan k_i z_i/\alpha_i \\ \alpha_i \tan k_i z_i & 0 \end{pmatrix}, \tag{11}$$

where $\boldsymbol{\Lambda}_i$ need not (and often cannot) be computed; for any scalar function f,

$$\boldsymbol{f}(\boldsymbol{\Lambda}_i) = \boldsymbol{M}_i \begin{pmatrix} f(k_i) & 0 \\ 0 & f(-k_i) \end{pmatrix} \boldsymbol{M}_i^{-1}. \tag{12}$$

In the matrix notation, Eqs. (4)–(9), all the boundary conditions are given by the $2N \times 2N$ complex, non-Hermitian matrix[22]

$$\begin{pmatrix} \exp(i\boldsymbol{\Lambda}_1 z_1) & -\exp(i\boldsymbol{\Lambda}_2 z_1) & 0 & \cdots & 0 & 0 \\ 0 & \exp(i\boldsymbol{\Lambda}_2 z_2) & -\exp(i\boldsymbol{\Lambda}_3 z_2) & \ddots & 0 & 0 \\ 0 & 0 & \exp(i\boldsymbol{\Lambda}_3 z_3) & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & \ddots & \exp(i\boldsymbol{\Lambda}_{N-1} z_{N-1}) & -\exp(i\boldsymbol{\Lambda}_N z_{N-1}) \\ -\exp(i\boldsymbol{\Lambda}_1 z_0 + iqd\boldsymbol{I}_2) & 0 & 0 & \cdots & 0 & \exp(i\boldsymbol{\Lambda}_N z_N) \end{pmatrix} \begin{pmatrix} \boldsymbol{D}_1 \\ \boldsymbol{D}_2 \\ \boldsymbol{D}_3 \\ \vdots \\ \boldsymbol{D}_{N-1} \\ \boldsymbol{D}_N \end{pmatrix} = 0, \tag{13}$$

where $\boldsymbol{D}_i = \boldsymbol{M}_i \boldsymbol{C}_i$ and all entries are 2×2 block matrices [see Eq. (10)]. The resulting eigenvector-eigenvalue problem will be solved in two ways: (a) in the exponential form, Eq. (13), which will lead to a generalized KP equation, Sec. III, or (b) by replacing the exponentials by tangents, which will lead to forms and geometric representations derived in Secs. IV–VII.

III. GENERALIZED KRONIG-PENNEY MODEL

Here, the well-known KP equation is derived in an algorithmically simple form. In Eq. (13), solving for $\boldsymbol{D}_2$ in terms of $\boldsymbol{D}_1$, $\boldsymbol{D}_3$ in terms of $\boldsymbol{D}_2$, etc., leads to the condition

$$[\exp(i\boldsymbol{\Omega} d) - \exp(iqd\boldsymbol{I}_2)]\boldsymbol{D}_1 = 0, \tag{14}$$

where

$$\exp(i\mathbf{\Omega}d) \equiv \exp(2i\mathbf{\Lambda}_N a_N) \cdots \exp(2i\mathbf{\Lambda}_2 a_2)\exp(2i\mathbf{\Lambda}_1 a_1) \tag{15}$$

and $\boldsymbol{I}_2$ is the 2×2 unit matrix. The matrix exponentials, Eq. (10), do not commute and $\mathbf{\Omega}$ is not Hermitian. Equation (14) is equivalent to the standard transfer matrix formulation,[12] and Eq. (15) is the transfer matrix. Solving Eq. (13) in the reverse order results in

$$[\exp(-iqd\boldsymbol{I}_2) - \exp(-i\mathbf{\Omega}d)]\boldsymbol{D}_N = 0, \tag{16}$$

where

$$\exp(-i\mathbf{\Omega}d) \equiv \exp(-2i\mathbf{\Lambda}_1 a_1) \times \exp(-2i\mathbf{\Lambda}_2 a_2) \cdots \exp(-2i\mathbf{\Lambda}_N a_N). \tag{17}$$

For nontrivial solutions of Eqs. (14) and (16), the determinants

$$\|\exp(i\mathbf{\Omega}d) - \boldsymbol{I}_2 \exp(iqd)\| = 0, \tag{18}$$

$$\|\boldsymbol{I}_2 \exp(-iqd) - \exp(-i\mathbf{\Omega}d)\| = 0. \tag{19}$$

Also, from time-reversal symmetry[10–12] $q\to -q$, Eq. (18) can be rewritten as

$$\|\exp(iqd)\exp(i\mathbf{\Omega}d) - \boldsymbol{I}_2\| = 0. \tag{20}$$

Multiplication of Eqs. (19) and (21) provides the generalized N-layer KP equation[24]

$$\|\cos \mathbf{\Omega}d - \boldsymbol{I}_2 \cos qd\| = 0, \tag{21}$$

where the matrix cosine[22,23]

$$\cos \mathbf{\Omega}d = [\exp(i\mathbf{\Omega}d) + \exp(-i\mathbf{\Omega}d)]/2. \tag{22}$$

In principle, Eq. (21) solves the problem; in practice, $\mathbf{\Omega}$ must be found from (15) by multiplying N noncommuting matrix exponentials, Eq. (10), as shown in the next section.

The KP equation (21) is particularly useful in finding eigenvalues but even for $N=2$ it provides no information about their parity. Also, to find eigenvectors, one must revert back to the full $2N\times 2N$ equation (13). The present formulation provides an alternative solution that is devoid of these problems.

Illustration

The cosine matrix $\cos \mathbf{\Omega}d = [\exp(i\mathbf{\Omega}d)+\exp(-i\mathbf{\Omega}d)]/2$ can be evaluated for any N by using the definition of the matrix exponential, Eq. (10)—i.e.,

$$\exp(i\mathbf{\Omega}d) = \prod_{i=1}^{N} \exp(2i\mathbf{\Lambda}_i a_i) = \prod_{i=1}^{N} \begin{pmatrix} c_i & is_i/\alpha_i \\ i\alpha_i s_i & c_i \end{pmatrix}, \tag{23}$$

where $c_i=\cos 2k_i a_i$ and $s_i=\sin 2k_i a_i$, and the order of multiplication is as in Eqs. (15) and (17). For example, for a two-layer PBG, the required products lead to the classic KP equation[10]

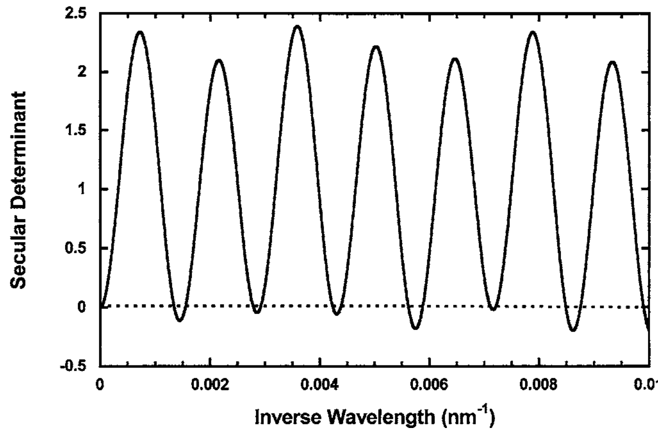

FIG. 1. The plot of the standard KP eigenfrequency condition, Eq. (28), at $q=0$ versus inverse wavelength for a three layer PBG material with $a_1=25.25$ nm, $a_2=75.2$ nm, $a_3=50.15$ nm, $n_1=2.33$, $n_2=1.45$, and $n_3=3.6$. Eigenfrequencies are found at the zeroes of the graph.

$$\cos qd = c_1c_2 - \left(\frac{\alpha_1}{\alpha_2} + \frac{\alpha_2}{\alpha_1}\right)\frac{s_1s_2}{2}. \tag{24}$$

The tangent form of Eq. (24) is[22,23]

$$\lfloor \tau_1^+/\alpha_1 + \tau_2/\alpha_2 \rfloor \times \lfloor \alpha_1\tau_1^- + \alpha_2\tau_2 \rfloor + \lfloor \tau_1^-/\alpha_1 + \tau_2/\alpha_2 \rfloor \times \lfloor \alpha_1\tau_1^+ + \alpha_2\tau_2 \rfloor = 0 \tag{25a}$$

or

$$\left\| \begin{matrix} \delta\tau_1 & \bar{\tau}_1/\alpha_1 + \tau_2/\alpha_2 \\ \alpha_1\bar{\tau}_1 + \alpha_2\tau_2 & \delta\tau_1 \end{matrix} \right\| = 0, \tag{25b}$$

where $\tau_1^{\pm}=\tan(k_1a_1 \pm qd/2)$, $\tau_i=\tan(k_ia_i)$, $\bar{\tau}_1=(\tau_1^- + \tau_1^+)/2$, and $\delta\tau_1=(\tau_1^- - \tau_1^+)/2$; at symmetry points $q=0,\pm\pi/d$, the tangents $\tau_1^+=\tau_1^-$, so that the tangent form is

$$[\tau_1/\alpha_1 + \tau_2/\alpha_2]\times[\alpha_1\tau_1 + \alpha_2\tau_2] = 0, \quad q=0, \tag{26}$$

$$[1/\alpha_1\tau_1 - \tau_2/\alpha_2]\times[\alpha_1/\tau_1 - \alpha_2\tau_2] = 0, \quad q = \pm\pi/d, \tag{27}$$

where the first (second) brackets are the conditions for the even (odd) parity eigenvalues, respectively, for the two-layer PBG.[10,25–27] In addition, the columns and rows of Eq. (25b) can be viewed as two-dimensional vectors and the eigenvalue condition as the requirement that the two vectors be collinear. This is the *first* instance of a geometric representation of an eigenfrequency condition. Clearly, even for $N=2$, the tangent formulation has a number of attractive features.

For a three-layer PBG, the multiplication of three matrices in Eq. (23) gives[4]

$$\cos qd = c_1c_2c_3 - \left(\frac{\alpha_1}{\alpha_2} + \frac{\alpha_2}{\alpha_1}\right)\frac{s_1s_2c_3}{2} - \left(\frac{\alpha_1}{\alpha_3} + \frac{\alpha_3}{\alpha_1}\right)\frac{s_1c_2s_3}{2} - \left(\frac{\alpha_2}{\alpha_3} + \frac{\alpha_3}{\alpha_2}\right)\frac{c_1s_2s_3}{2}, \tag{28}$$

which is invariant with respect to all permutations of layer indices. For greater N, the multiplication of N matrices leads to a multiterm expression that quickly becomes unwieldy, brings no additional insights, and does not reduce the computational effort. For future comparison, Fig. 1 plots Eq. (28) as a function of inverse wavelength for a three-layer PBG material at $q=0$.

The tangent form for a three-layer PBG can be derived from Eq. (23) by using trigonometric identities, and at $q=0$ it is given by

$$\tau_1^2\tau_2^2\tau_3^2+\tau_1^2+\tau_2^2+\tau_3^2-\tau_1^2\tau_2\tau_3\left(\frac{\alpha_2}{\alpha_3}+\frac{\alpha_3}{\alpha_2}\right)-\tau_1\tau_2^2\tau_3\left(\frac{\alpha_1}{\alpha_3}+\frac{\alpha_3}{\alpha_1}\right)-\tau_1\tau_2\tau_3^2\left(\frac{\alpha_1}{\alpha_2}+\frac{\alpha_2}{\alpha_1}\right)+\tau_1\tau_2\left(\frac{\alpha_1}{\alpha_2}+\frac{\alpha_2}{\alpha_1}\right)+\tau_1\tau_3\left(\frac{\alpha_1}{\alpha_3}+\frac{\alpha_3}{\alpha_1}\right)+\tau_2\tau_3\left(\frac{\alpha_2}{\alpha_3}+\frac{\alpha_3}{\alpha_2}\right)=0, \tag{29}$$

which while symmetric is not very illuminating, algorithmically convenient, or easily extendable to a greater number of layers or to a general q vector (however, at $q=\pm\pi/d$, replace $\tau_1\to-1/\tau_1$). Clearly, a more formal approach is necessary.

Observe that in the vacuum limit, $\alpha_i=1$, Eq. (29) can be factored as

$$(\tau_1\tau_2\tau_3-\tau_1-\tau_2-\tau_3)^2=0. \tag{30}$$

This is the "triangle condition" that is satisfied whenever the sum of the arguments of the three tangents, $k_1a_1+k_2a_2+k_3a_3=P\pi$ for integer $P\geqslant 0$, so that $\lambda=d/P$ at $q=0$. (A special case is the zero-frequency condition, $k_1=k_2=k_3=0$, for which $\tau_1=\tau_2=\tau_3=0$.) This condition corresponds to an artificial division of vacuum into slabs of width d and is independent of the individual layer widths.

It is the possibility of analytic forms and their geometric representations that motivates the development of the alternative formulation in Secs. IV–VII. In particular, in Sec. IV, Eq. (29) will be factored into two parts, Eq. (78), and analytic wave functions will be found.

IV. TANGENT FORMULATION FOR N LAYERS

A. Reformulated eigenvector-eigenvalue problem

By defining a new eigenvector

$$\boldsymbol{G}_i=\exp(i\boldsymbol{\Lambda}_i z_i)\boldsymbol{D}_i=\exp(i\boldsymbol{\Lambda}_i z_i)\boldsymbol{M}_i\boldsymbol{C}_i, \tag{31}$$

the secular equation (13) can be expressed in terms of layer widths

$$\begin{pmatrix} \boldsymbol{I}_2 & -\exp(-2i\boldsymbol{\Lambda}_2a_2) & 0 & \cdots & 0 & 0\\ 0 & \boldsymbol{I}_2 & -\exp(-2i\boldsymbol{\Lambda}_3a_3) & \ddots & 0 & 0\\ 0 & 0 & \ddots & \ddots\ \ddots & & 0\\ \vdots & \ddots & \ddots & \ddots\ \ddots & & \ddots\\ 0 & 0 & 0 & \ddots & \boldsymbol{I}_2 & -\exp(-2i\boldsymbol{\Lambda}_Na_N)\\ -\boldsymbol{I}_2\exp(-2i\boldsymbol{\Lambda}_1a_1+qd\boldsymbol{I}_2) & 0 & 0 & \cdots & 0 & \boldsymbol{I}_2 \end{pmatrix}\begin{pmatrix}\boldsymbol{G}_1\\ \boldsymbol{G}_2\\ \cdot\\ \cdot\\ \boldsymbol{G}_{N-1}\\ \boldsymbol{G}_N\end{pmatrix}=0. \tag{32}$$

Then, using the identity[11]

$$\exp(2i\boldsymbol{\Lambda}a_i)=(\boldsymbol{I}+i\tan\boldsymbol{\Lambda}a_i)/(\boldsymbol{I}-i\tan\boldsymbol{\Lambda}a_i), \tag{33}$$

all matrix exponentials turn into matrix tangents. For *odd N*, by row addition and subtraction, Eq. (32) can be rearranged as[22]

$$\begin{pmatrix} \tan(\boldsymbol{\Lambda}_1a_1-qd/2) & i\boldsymbol{I}_2 & -i\boldsymbol{I}_2 & \cdots & i\boldsymbol{I}_2 & -i\boldsymbol{I}_2\\ & \tan\boldsymbol{\Lambda}_2a_2 & i\boldsymbol{I}_2 & \ddots & -i\boldsymbol{I}_2 & i\boldsymbol{I}_2\\ & & \ddots & \ddots & \ddots & -i\boldsymbol{I}_2\\ & c.c. & & \ddots & \ddots & \ddots\\ & & & & \tan\boldsymbol{\Lambda}_{N-1}a_{N-1} & i\boldsymbol{I}_2\\ & & & & & \tan\boldsymbol{\Lambda}_Na_N \end{pmatrix}\begin{pmatrix}\boldsymbol{W}_1\\ \boldsymbol{W}_2\\ \cdot\\ \cdot\\ \boldsymbol{W}_{N-1}\\ \boldsymbol{W}_N\end{pmatrix}=0, \tag{34}$$

where

$$\boldsymbol{W}_i = \frac{\boldsymbol{I}}{\boldsymbol{I} + i\tan(\boldsymbol{\Lambda}_i a_i)}\boldsymbol{G}_i = \frac{\boldsymbol{I}}{\boldsymbol{I} + i\tan(\boldsymbol{\Lambda}_i a_i)}\exp(i\boldsymbol{\Lambda}_i z_i)\boldsymbol{M}_i\boldsymbol{C}_i, \quad i = 2, \ldots, N, \tag{35}$$

$$\boldsymbol{W}_1 = \frac{\boldsymbol{I}}{\boldsymbol{I} + i\tan(\boldsymbol{\Lambda}_1 a_1 - qd/2)}\boldsymbol{G}_1 = \frac{\boldsymbol{I}}{\boldsymbol{I} + i\tan(\boldsymbol{\Lambda}_1 a_1 - qd/2)}\exp(i\boldsymbol{\Lambda}_1 z_1)\boldsymbol{M}_1\boldsymbol{C}_1, \quad i = 1. \tag{36}$$

Conversely, once eigenvectors $\boldsymbol{W}_i$ are calculated, the wave amplitudes are found from

$$\boldsymbol{C}_i = \exp[-i\boldsymbol{K}_i(a_i + z_{i-1})]\sec(\boldsymbol{K}_i a_i)(\boldsymbol{M}_i^{-1}W_i), \quad i = 2, \ldots, N, \tag{37a}$$

$$\boldsymbol{C}_1 = \exp[-i(\boldsymbol{K}_1 a_1 + qd/2)]\sec(\boldsymbol{K}_1 a_1 - qd/2)(\boldsymbol{M}_1^{-1}\boldsymbol{W}_1), \quad i = 1. \tag{37b}$$

For N even, the relevant treatment is presented in Appendix B.[22] For the purposes of the present paper, the results for N even can be found by using the results for N odd in the limit of one the layer widths going to zero.

B. Main equation: Reduction to a 2×2 block form

For PBG's, the 2×2 tangent matrices, Eq. (11), are given by

$$\tan \boldsymbol{\Lambda}_i a_i = \begin{pmatrix} 0 & \tau_i/\alpha_i \\ \alpha_i\tau_i & 0 \end{pmatrix}, \tag{38a}$$

$$\tan(\boldsymbol{\Lambda}_1 a_1 - qd\boldsymbol{I}_2/2) = \frac{1}{2}\begin{pmatrix} \tau_1^- - \tau_1^+ & (\tau_1^- + \tau_1^+)/\alpha_1 \\ (\tau_1^- + \tau_1^+)\alpha_1 & \tau_1^- - \tau_1^+ \end{pmatrix} \equiv \begin{pmatrix} \delta\tau_1 & \bar{\tau}_1/\alpha_1 \\ \bar{\tau}_1\alpha_1 & \delta\tau_1 \end{pmatrix}, \tag{38b}$$

where

$$\bar{\tau}_1 = (\tau_1^+ + \tau_1^-)/2, \tag{39a}$$

$$\delta\tau_1 = (\tau_1^- - \tau_1^+)/2. \tag{39b}$$

Next, Eqs. (38a) and (38b) are substituted into the secular equation (34) and vector

$$\boldsymbol{W}_i = \begin{pmatrix} \boldsymbol{W}_i^+ \\ \boldsymbol{W}_i^- \end{pmatrix}$$

is split into its upper and lower components. After further rearrangement, the $2N\times 2N$ secular equation can be written as a 2×2 matrix of $N\times N$ block matrices, henceforth called the *main equation*, the central result of the present paper,

$$\begin{pmatrix} \boldsymbol{TA} & \boldsymbol{J} \\ \boldsymbol{J} & \boldsymbol{TA}^{-1} \end{pmatrix}\begin{pmatrix} \boldsymbol{W}^+ \\ \boldsymbol{W}^- \end{pmatrix} \equiv \boldsymbol{\Phi}(\boldsymbol{A})\begin{pmatrix} \boldsymbol{W}^+ \\ \boldsymbol{W}^- \end{pmatrix} = \boldsymbol{0}. \tag{40}$$

For odd N, the $N\times N$ matrices $\boldsymbol{T}$ and $\boldsymbol{A}$ are real diagonal and given by

$$\mathbf{T} = \begin{pmatrix} \bar{\tau}_1 & 0 & 0 & \cdots & 0 \\ 0 & \tau_2 & 0 & \ddots & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & 0 & \tau_{N-1} & 0 \\ 0 & 0 & \cdots & 0 & \tau_N \end{pmatrix}, \tag{41}$$

$$\boldsymbol{A} = \begin{pmatrix} \alpha_1 & 0 & 0 & \cdots & 0 \\ 0 & \alpha_2 & 0 & \ddots & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & 0 & \alpha_{N-1} & 0 \\ 0 & 0 & \cdots & 0 & \alpha_N \end{pmatrix}, \tag{42}$$

and the $N\times N$ Hermitian matrix $\boldsymbol{J}$ is given by

$$\boldsymbol{J} = \begin{pmatrix} \delta\tau_1 & i & -i & \cdots & i & -i \\ -i & 0 & i & \ddots & -i & i \\ i & -i & 0 & \ddots & \ddots & -i \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ -i & i & \ddots & \ddots & 0 & i \\ i & -i & i & \cdots & -i & 0 \end{pmatrix}. \tag{43}$$

The developments below are all the consequences of the main equation (40), which has the form of the operator Riccati equation.[13–17] Observe that at symmetry points, $\delta\tau_1=0$, and $\boldsymbol{J}$ is i times a real skew-symmetric matrix (i.e., its determinant is zero). The simplicity of the main equation, the diagonality of $\boldsymbol{T}$ and $\boldsymbol{A}$, and the Hermiticity of $\boldsymbol{J}$ make possible the analytic progress below.

C. Properties of the main equation

The reduction of the $2N\times 2N$ secular equation to the 2×2 secular matrix of $N\times N$ block matrices, Eq. (40), simplifies the problem mathematically and conceptually. Since $\boldsymbol{T}$, $\boldsymbol{A}$, and $\boldsymbol{J}$, are all Hermitian, the secular matrix is also Hermitian,

$$\boldsymbol{\Phi}(\boldsymbol{A})^{\dagger} = \boldsymbol{\Phi}(\boldsymbol{A}), \tag{44}$$

and its determinant is real. By contrast, in the KP formulation, Eqs. (13) is non-Hermitian. Moreover, with $\boldsymbol{T}$ held constant, the determinant is invariant under the interchange

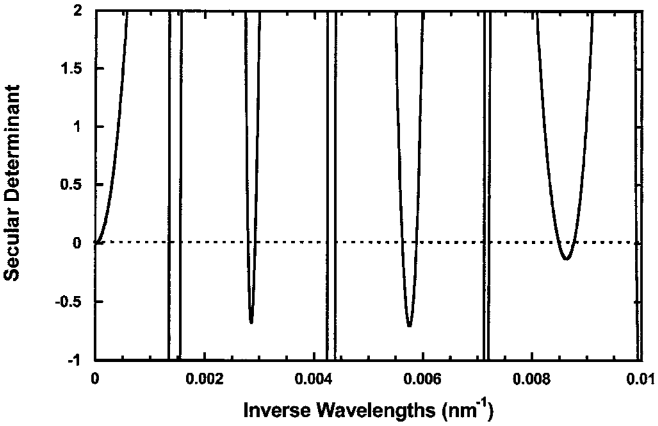

FIG. 2. The 6×6 secular determinant of the main equation, Eq. (40), $\|\mathbf{\Phi}\{\boldsymbol{A}\}\|$, for the three-layer case of Fig. 1. Eigenfrequencies at the zeros of the graph coincide with those of Fig. 1. Singularities due to the tangents can be eliminated by multiplying the graph by the corresponding cosines.

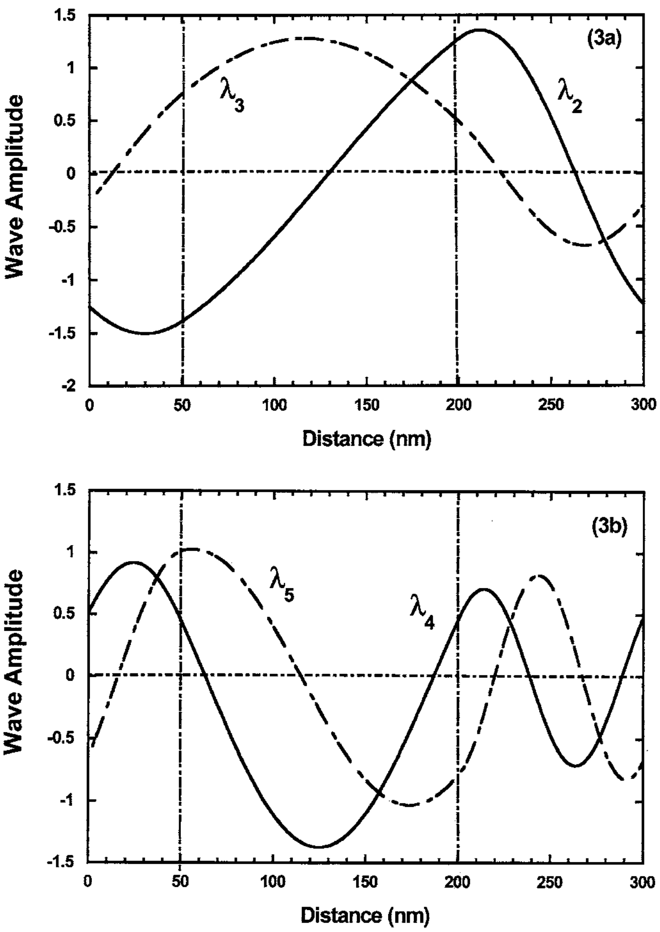

FIG. 3. The wave functions for the lowest two (a) and next two lowest (b) eigenfrequencies calculated with Eq. (40) for the case of the three-layer PBG of Fig. 1 at $q=0$. Here $1/\lambda_2=0.00134661\ \text{nm}^{-1}$, $1/\lambda_3=0.00154943\ \text{nm}^{-1}$, $1/\lambda_4=0.00279033\ \text{nm}^{-1}$, and $1/\lambda_5=0.00291967\ \text{nm}^{-1}$.

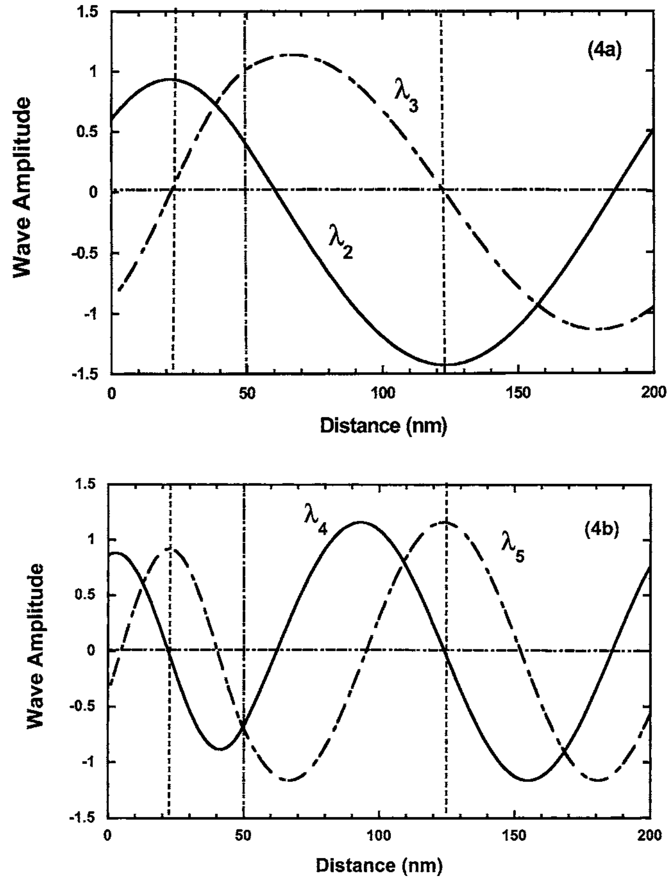

FIG. 4. The corresponding wave functions for the lowest two (a) and next two lowest (b) eigenfrequencies calculated with Eq. (40) by setting $a_3=0$. The three-layer wave functions, Fig. 3, are seen to evolve from those of Fig. 4, while retaining the same node pattern. Here, $1/\lambda_2=0.0028066\ \text{nm}^{-1}$, $1/\lambda_3=0.0031652\ \text{nm}^{-1}$, $1/\lambda_4=0.0057406\ \text{nm}^{-1}$, and $1/\lambda_5=0.0061640\ \text{nm}^{-1}$.

$\boldsymbol{A}\leftrightarrow\boldsymbol{A}^{-1}$—i.e., as a functional of $\boldsymbol{A}$:

$$\|\mathbf{\Phi}\{\boldsymbol{A}\}\| = \|\mathbf{\Phi}\{\boldsymbol{A}^{-1}\}\|. \tag{45}$$

Since $\mathbf{\Phi}(\boldsymbol{A})$ is Hermitian, it can be diagonalized by a unitary transformation $\boldsymbol{U}\mathbf{\Phi}(\boldsymbol{U})^{-1}=\mathbf{\Gamma}$, producing $2N$ real eigenvalues Γ_{ii} and N orthonormal eigenvectors $\boldsymbol{U}_i$. At an eigenfrequency, one of the eigenvalues $\Gamma_{jj}=0$, $1\le j\le N$; the corresponding eigenvector $\boldsymbol{U}_j=\boldsymbol{W}$ furnishes the wave function amplitudes $\boldsymbol{W}^{\pm}$, Eqs. (35) and (36), which in turn can be used to find the forward/backward amplitudes $c^{\pm}$ via Eq. (37) and ultimately the wave functions themselves, Eq. (3).

For the three-layer case of Fig. 1, $\|\mathbf{\Phi}\{\boldsymbol{A}\}\|$ is a 6×6 determinant and is plotted in Fig. 2. The horizontal axis intercepts are seen to produce the same eigenfrequencies as in Fig. 1 to within computer accuracy. At $q=0$ and $N=3$, the 6×6 determinant $\|\mathbf{\Phi}\{\boldsymbol{A}\}\|$ can be evaluated analytically and indeed is given by Eq. (29); here, however, $\|\mathbf{\Phi}\{\boldsymbol{A}\}\|$ has been derived using a consistent, generalized procedure. The corresponding wave functions for a few lowest (nonzero)

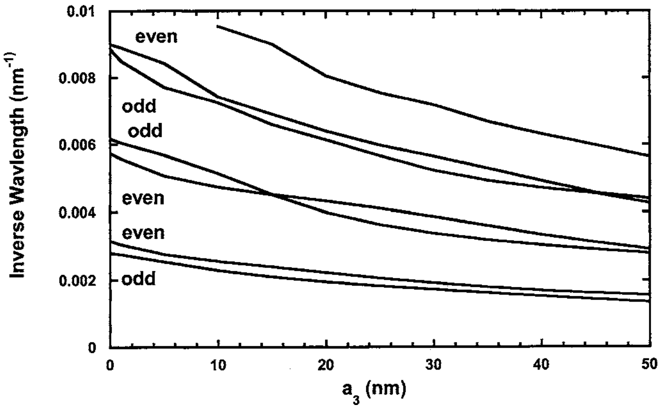

FIG. 5. The evolution of the bands for the PBG of Fig. 1 as a function of a_3, calculated with the use of Eq. (40). On finer scale, the bands anticross.

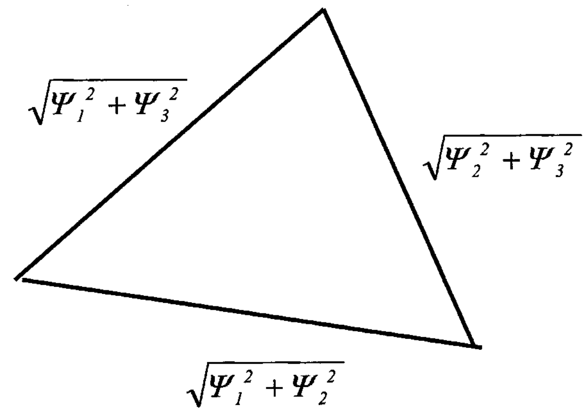

FIG. 6. The triangle whose sides, Eq. (52c), satisfy the eigenfrequency conditions for a three-layer PBG at $q=0$ as long as $\Psi_1\Psi_2\Psi_3+\Psi_1\Psi_2+\Psi_1\Psi_3+\Psi_2\Psi_3=0$, which requires the triangle to lie on a plane passing through the origin of the coordinate system.

eigenfrequencies of the main equation are shown in Figs. 3(a) and 3(b). These wave functions evolve continuously from those for two-layer PBG's, Figs. 4(a) and 4(b), which were also obtained from the main equation by setting one layer width (here, a_3) to zero. The order of the eigenfrequencies, parities, and node numbers for the two-layer PBG is (1) even/odd with two nodes, Fig. 4(a); (2) odd/even with four nodes, Fig. 4(b); (3) even/odd with six nodes, etc., where the parity is with respect to the centers of each layer. In Figs. 3(a) and 3(b), the three-layer wave functions lack parity, but by continuity they preserve the number of nodes so that eigenfrequencies also occur in pairs with the same (even) number of nodes—that is, two nodes for (λ_2,λ_3), four nodes for (λ_4,λ_5), etc. The evolution of the bands as a function of a_3 is shown in Fig. 5, where (on a finer scale) the bands exhibit a number of avoided crossings.

These examples demonstrate the equivalence of the present and the standard KP formalisms and the ease of application of the main equation to the N-layer KP problem for both eigenfrequency and wave function calculations. However, in Secs. V–VII below, the problem is further simplified.

V. REDUCTION TO $N\times N$ FORM

A. Determinant

The size of the determinant of the main equation (40) can be halved using determinant identities on block matrices.[28,29] If $\boldsymbol{TA}$ is invertible [that is, if $\bar{\tau}_1\neq 0$ and $\tau_i\neq 0$, in Eq. (41)], the secular determinant is given by

$$\|\Phi\{A\}\| = \|\boldsymbol{TA}\| \times \|\boldsymbol{TA}^{-1} - \boldsymbol{J}(\boldsymbol{TA})^{-1}\boldsymbol{J}\|, \tag{46}$$

where for a nontrivial solution Schur complement (the second factor) must be zero. The determinant $\|\boldsymbol{TA}\|$ in front cancels the singularities due to the matrix inverse $(\boldsymbol{TA})^{-1}$; singularities due to the tangents themselves are removable by multiplying by the corresponding cosines. Equation (46) remains valid in the limit of any (but not at) $\tau_i=0$. Being an identity, Eq. (46) yields results identical to those in Fig. 2.

B. Explicit form for odd N

For general, odd N, performing the matrix multiplication in Eq. (46), the resulting determinant has the Hermitian form shown here for $N=5$,

$$(\bar{\zeta}_1\zeta_2\zeta_3\zeta_4\zeta_5)\left\|\begin{matrix} \left(\bar{\xi}_1-\frac{(\delta\tau_1)^2}{\bar{\zeta}_1}\right)-\Sigma_{11} & -\frac{i\delta\tau_1}{\bar{\zeta}_1}+\Sigma_{12} & \frac{i\delta\tau_1}{\bar{\zeta}_1}+\Sigma_{13} & -\frac{i\delta\tau_1}{\bar{\zeta}_1}+\Sigma_{14} & \frac{i\delta\tau_1}{\bar{\zeta}_1}+\Sigma_{15} \\ & \xi_2-\Sigma_{22} & \Sigma_{23} & \Sigma_{24} & \Sigma_{25} \\ & & \xi_3-\Sigma_{33} & \Sigma_{34} & \Sigma_{35} \\ & c.c. & & \xi_4-\Sigma_{44} & \Sigma_{45} \\ & & & & \xi_5-\Sigma_{55} \end{matrix}\right\| = 0, \tag{47}$$

where c.c. indicates complex conjugation, $\zeta_i=\alpha_i\tau_i$, $\xi_i=\tau_i/\alpha_i$, and

$$\Sigma_{ij} = \sum_{k\neq i,j}^{5} \zeta_k^{-1}; \tag{48}$$

extensions to higher, odd N are clear. Terms of order $\delta\tau_1$ are odd functions of q and so must vanish. Expanding the determinant, one finds

$$(\bar{\zeta}_1\zeta_2\zeta_3\zeta_4\zeta_5)\left\|\begin{matrix} \left(\bar{\xi}_1-\frac{(\delta\tau_1)^2}{\bar{\zeta}_1}\right)-\Sigma_{11} & \Sigma_{12} & \Sigma_{13} & \Sigma_{14} & \Sigma_{15} \\ \Sigma_{12} & \xi_2-\Sigma_{22} & \Sigma_{23} & \Sigma_{24} & \Sigma_{25} \\ \Sigma_{13} & \Sigma_{23} & \xi_3-\Sigma_{33} & \Sigma_{34} & \Sigma_{35} \\ \Sigma_{14} & \Sigma_{24} & \Sigma_{34} & \xi_4-\Sigma_{44} & \Sigma_{45} \\ \Sigma_{15} & \Sigma_{25} & \Sigma_{35} & \Sigma_{45} & \xi_5-\Sigma_{55} \end{matrix}\right\| + (\bar{\zeta}_1\zeta_2\zeta_3\zeta_4\zeta_5)\left(\frac{\delta\tau_1}{\bar{\zeta}_1}\right)^2\left\|\begin{matrix} 0 & 1 & -1 & 1 & -1 \\ 1 & \xi_2-\Sigma_{22} & \Sigma_{23} & \Sigma_{24} & \Sigma_{25} \\ -1 & \Sigma_{23} & \xi_3-\Sigma_{33} & \Sigma_{34} & \Sigma_{35} \\ 1 & \Sigma_{24} & \Sigma_{34} & \xi_4-\Sigma_{44} & \Sigma_{45} \\ -1 & \Sigma_{25} & \Sigma_{35} & \Sigma_{45} & \xi_5-\Sigma_{55} \end{matrix}\right\| = 0, \tag{49a}$$

where all the matrices are real symmetric. This form, just as the submain equation (46), is algorithmically simple and suitable for machine calculations. For $q=0$, the tangent difference $\delta\tau_1=0$ so that from Eq. (49a), the columns and rows of the determinant matrix

$$(\zeta_1\zeta_2\zeta_3\zeta_4\zeta_5) \times \left\|\begin{matrix} \xi_1-\Sigma_{11} & \Sigma_{12} & \Sigma_{13} & \Sigma_{14} & \Sigma_{15} \\ \Sigma_{12} & \xi_2-\Sigma_{22} & \Sigma_{23} & \Sigma_{24} & \Sigma_{25} \\ \Sigma_{13} & \Sigma_{23} & \xi_3-\Sigma_{33} & \Sigma_{34} & \Sigma_{35} \\ \Sigma_{14} & \Sigma_{24} & \Sigma_{34} & \xi_4-\Sigma_{44} & \Sigma_{45} \\ \Sigma_{15} & \Sigma_{25} & \Sigma_{35} & \Sigma_{45} & \xi_5-\Sigma_{55} \end{matrix}\right\| = 0 \tag{49b}$$

can be viewed as vectors in a five-dimensional space, with their termini describing a five-sided figure. The eigenfrequency condition, Eq. (49b), then dictates that one of the vectors be linearly dependent on the other four vectors, so that the five-sided figure lies in a four-dimensional space. A case for $N=3$ is demonstrated next.

C. Analytic and graphical representation for $N=3$ at $q=0,\pm\pi/d$

For $N=3$ and $q=0$, Eq. (46) or (49b) yields

$$\|\mathbf{\Phi}\{\boldsymbol{A}\}\| = \frac{1}{\zeta_1\zeta_2\zeta_3}\left\|\begin{matrix} \xi_1\zeta_3\zeta_2-\zeta_3-\zeta_2 & \zeta_2 & \zeta_3 \\ \zeta_1 & \xi_2\zeta_1\zeta_3-\zeta_3-\zeta_1 & \zeta_3 \\ \zeta_1 & \zeta_2 & \xi_3\zeta_1\zeta_2-\zeta_1-\zeta_2 \end{matrix}\right\| \tag{50a}$$

or

$$\left\|\begin{matrix} \Theta_1 & 1 & 1 \\ 1 & \Theta_2 & 1 \\ 1 & 1 & \Theta_3 \end{matrix}\right\| = (\Theta_1\Theta_2\Theta_3-\Theta_1-\Theta_2-\Theta_3+2)=0, \tag{50b}$$

where $\Theta_1=(\xi_1\zeta_3\zeta_2-\zeta_2-\zeta_3)/\zeta_1=[(\tau_1/\alpha_1)(\tau_2\alpha_2)(\tau_3\alpha_3)-\tau_2\alpha_2-\tau_3\alpha_3]/(\tau_1\alpha_1)$, etc. Here, the eigenvalue condition, Eq. (50b), requires that the three vectors $(\Theta_1\ 1\ 1)$, $(1\ \Theta_2\ 1)$, and $(1\ 1\ \Theta_3)$ be coplanar. The three vectors define a planar triangle in a plane through the origin of the coordinate system, an appealing geometric representation for a three-layer problem [also see Fig. 6 following the discussion of Eqs. (52a)–(52c)]. At an eigenfrequency, the condition $(\Theta_1\Theta_2\Theta_3-\Theta_1-\Theta_2-\Theta_3+2)=0$ is satisfied by two sets of $(\Theta_1,\Theta_2,\Theta_3)$, with one obtained from the other by the replacement $\boldsymbol{A}\to\boldsymbol{A}^{-1}$.

In the vacuum limit $\alpha_i=1$, the $N=3$ expression, Eq. (50a), becomes

$$\|\mathbf{\Phi}\{A\}\| = \frac{1}{\tau_1\tau_2\tau_3}\begin{Vmatrix} \tau_1\tau_3\tau_2 - \tau_3 - \tau_2 & \tau_2 & \tau_3 \\ \tau_1 & \tau_2\tau_1\tau_3 - \tau_3 - \tau_1 & \tau_3 \\ \tau_1 & \tau_2 & \tau_3\tau_1\tau_2 - \tau_1 - \tau_2 \end{Vmatrix} = (\tau_1\tau_2\tau_3 - \tau_1 - \tau_2 - \tau_3)^2 \qquad (51)$$

and was already discussed in connection with Eq. (30), but here it is derived systematically.

Another symmetric expression is found by rewriting Eq. (50a) as

$$\|\mathbf{\Phi}\{A\}\| = \frac{1}{\zeta_1\zeta_2\zeta_3}\begin{Vmatrix} (\xi_1\zeta_3\zeta_2 - \zeta_3 - \zeta_2 - \zeta_1) + \zeta_1 & \zeta_2 & \zeta_3 \\ \zeta_1 & (\xi_2\zeta_1\zeta_3 - \zeta_1 - \zeta_2 - \zeta_3) + \zeta_2 & \zeta_3 \\ \zeta_1 & \zeta_2 & (\xi_3\zeta_1\zeta_2 - \zeta_1 - \zeta_2 - \zeta_3) + \zeta_3 \end{Vmatrix}$$

$$= \begin{Vmatrix} 1+\Psi_1 & 1 & 1 \\ 1 & 1+\Psi_2 & 1 \\ 1 & 1 & 1+\Psi_3 \end{Vmatrix} = 0, \qquad (52a)$$

so that

$$\|\mathbf{\Phi}\{A\}\| = \Psi_1\Psi_2\Psi_3 + \Psi_1\Psi_2 + \Psi_1\Psi_3 + \Psi_2\Psi_3 = 0, \qquad (52b)$$

where

$$\Psi_1 = (\xi_1\zeta_3\zeta_2 - \zeta_1 - \zeta_2 - \zeta_3)/\zeta_1,$$

$$\Psi_2 = (\xi_2\zeta_1\zeta_3 - \zeta_1 - \zeta_2 - \zeta_3)/\zeta_2,$$

$$\Psi_3 = (\xi_3\zeta_1\zeta_2 - \zeta_1 - \zeta_2 - \zeta_3)/\zeta_3. \qquad (52c)$$

The eigenfrequency condition, Eq. (52b), is a graph of a plane in three dimensions that can be plotted in the natural units of ζ_1, ζ_2, and ζ_3. Conversely, this condition requires that the column and row vectors be coplanar so that one of the column or row vectors of Eq. (52b) can be written as a linear combination of the other two—i.e.,

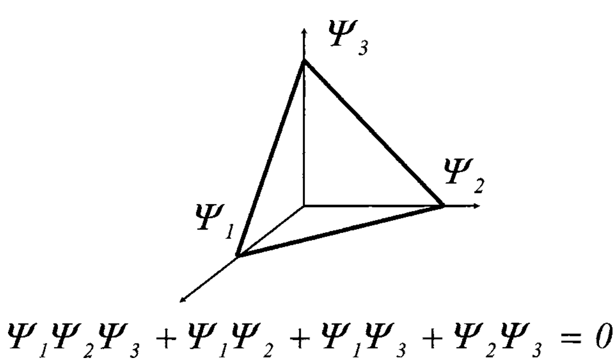

FIG. 7. The upper face of this tetrahedron is the triangle of Fig. 6 whose sides satisfy the eigenfrequency conditions for a three-layer PBG at $q=0$. The coordinate system is offset by (1,1,1) from the true origin.

$$\begin{pmatrix} 1 \\ 1 \\ 1+\Psi_3 \end{pmatrix} = p_1\begin{pmatrix} 1+\Psi_1 \\ 1 \\ 1 \end{pmatrix} + p_2\begin{pmatrix} 1 \\ 1+\Psi_2 \\ 1 \end{pmatrix}, \qquad (53)$$

which has the solution

$$p_1 = \frac{\Psi_2}{\Psi_1 + \Psi_2 + \Psi_1\Psi_2}, \quad p_2 = \frac{\Psi_1}{\Psi_1 + \Psi_2 + \Psi_1\Psi_2}, \qquad (54)$$

as long as Eq. (52b) is true.

The triangle representing the eigenfrequency condition is plotted in Fig. 6 and the lengths of its sides depend on frequencies through the tangents that define Ψ's, Eq. (52c). For $q=\pi/d$, replace τ_1 by $\tan(k_1a_1 \pm \pi/2) = -1/\tau_1$. The conditions on the lengths of the sides of the triangle, Fig. 6, are incorporated into the tetrahedron figure, Fig. 7. The eigenvalue condition requires that the triangular face pass through the origin of the coordinate system. A similar construction exists for $N>3$ in N-dimensional space.

Although Eq. (46) was derived assuming the invertibility

TABLE I. Comparison of the inverse wavelengths for the three-layer example of Fig. 1 calculated using the 3×3 expression, Eq. (46), with $a_3=0.01$ nm versus the 6×6 expression, Eq. (40), with $a_3=0$ nm, showing that the formalism is accurate in the limit of $N=2$. Here, $a_1=25.25$ nm, $a_2=75.2$ nm, $n_1=2.33$, and $n_2=1.45$.

Inverse wavelengths (nm^{-1}) using Eq. (46) with $a_3=0.01$ nm	Inverse wavelengths (nm^{-1}) using Eq. (40) with $a_3=0$ nm
0.0028062	0.0028066
0.0031641	0.0031652
0.0057389	0.0057406
0.0061628	0.0061640
0.0088565	0.0088603
0.0090001	0.0090011

of Eq. (41), the formalism remains valid in the limit of any $\tau_i \to 0$. For example, numerical tests with $\tau_3 \to 0$ (by setting $a_3=0.01$ nm) returned eigenfrequencies within 0.1% of the two-layer result ($a_3=0$ nm), Table I. Indeed, in the limit of $\tau_3 \to 0$, the three-layer expression, Eq. (50a) can be expanded to $O(\tau_3)$, after which τ_3 can be set to zero. This procedure results in the correct two-layer limit, Eqs. (26) and (27),

$$(\zeta_1+\zeta_2)(\xi_1+\xi_2)=(\alpha_1\tau_1+\alpha_2\tau_1)(\tau_1/\alpha_1+\tau_1/\alpha_2)=0, \tag{55}$$

where the first (second) brackets are the conditions for odd (even) parity eigenstates; the conditions

$$\zeta_1+\zeta_2=0, \tag{56}$$

$$\xi_1+\xi_2=0 \tag{57}$$

are equations of lines in two-dimensional space.

VI. $N\times N$ EIGENVECTOR AND EIGENVALUE EQUATION

Section V dealt only with the secular determinant and calculations of eigenfrequencies; here, the complete $N\times N$ eigenvector and eigenvalue equation is derived from the main equation. From the top row of Eq. (40),

$$\boldsymbol{W}^+=-(\boldsymbol{TA})^{-1}\boldsymbol{JW}^-, \tag{58a}$$

which when substituted into the bottom row yields

$$\left(\frac{\boldsymbol{T}}{\boldsymbol{A}}-\boldsymbol{J}\frac{\boldsymbol{I}}{\boldsymbol{AT}}\boldsymbol{J}\right)\boldsymbol{W}^-=\boldsymbol{0}; \tag{59a}$$

similarly, from the bottom row of Eq. (40),

$$\boldsymbol{W}^-=-\frac{\boldsymbol{A}}{\boldsymbol{T}}\boldsymbol{JW}^+, \tag{58$'$}$$

which when substituted into the top row gives

$$\left(\boldsymbol{TA}-\boldsymbol{J}\frac{\boldsymbol{A}}{\boldsymbol{T}}\boldsymbol{J}\right)\boldsymbol{W}^+=\boldsymbol{0}. \tag{59$'$}$$

These constitute two separate eigenvalue-eigenvector problems for the up and down vector components and will be called the *submain equations*. These equations have the following properties: (a) they are Hermitian, (b) the secular determinants are related since

$$\left\|\begin{matrix}\boldsymbol{AT} & \boldsymbol{J}\\ \boldsymbol{J} & \dfrac{\boldsymbol{T}}{\boldsymbol{A}}\end{matrix}\right\| = \left\|\frac{\boldsymbol{T}}{\boldsymbol{A}}\right\|\times\left\|\boldsymbol{AT}-\boldsymbol{J}\frac{\boldsymbol{A}}{\boldsymbol{T}}\boldsymbol{J}\right\| = \|\boldsymbol{AT}\|\times\left\|\frac{\boldsymbol{T}}{\boldsymbol{A}}-\boldsymbol{J}\frac{\boldsymbol{I}}{\boldsymbol{AT}}\boldsymbol{J}\right\|=0, \tag{60}$$

and so they produce the same eigenfrequency spectrum, (c) the size of the secular equation has been halved from $2N\times 2N$ to $N\times N$, and (d) the eigenvectors of Eqs. (59a) and (59′) are related by Eqs. (58a) and (58′) so that only one submain equations need be solved.

As an example of the use of the submain equation, the full band structure for the case of Fig. 1 is calculated by diagonalizing Eq. (59a) and is shown as Fig. 8. The eigenvector of Eq. (59a) corresponding to the zero eigenvalue is $\boldsymbol{W}^-$; the corresponding $\boldsymbol{W}^+$ is then found from Eq. (58a). The wave functions calculated with these eigenvectors are indistinguishable from those in Figs. 3(a) and 3(b).

Because of the twofold reduction in size, the present formalism is amenable to further analytical development, most importantly the diagonalization of the submain equation. The procedure will be demonstrated on the example of a $N=3$ PBG by deriving analytic eigenfrequency conditions and wave functions.

VII. DIAGONALIZATION OF THE SUBMAIN EQUATION, CALCULATION OF EIGENFREQUENCIES, AND ANALYTIC WAVE FUNCTIONS

A. Further simplifications

For further developments, it is easier to use the $N\times N$ matrices

$$\boldsymbol{X}=\left(\frac{\boldsymbol{A}}{\boldsymbol{T}}\right)^{1/2}\boldsymbol{J}\frac{\boldsymbol{I}_N}{(\boldsymbol{TA})^{1/2}}, \tag{61}$$

$$\bar{\boldsymbol{X}}=\frac{\boldsymbol{I}_N}{(\boldsymbol{TA})^{1/2}}\boldsymbol{J}\left(\frac{\boldsymbol{A}}{\boldsymbol{T}}\right)^{1/2}, \tag{62}$$

in terms of which Eq. (46) assumes the simple form

$$\|\boldsymbol{\Phi}\{\boldsymbol{A}\}\|=\|\boldsymbol{T}\|^2\times\|\boldsymbol{I}-\boldsymbol{X}\bar{\boldsymbol{X}}\|. \tag{63}$$

Since $\boldsymbol{T}$ can have negative elements, $\bar{\boldsymbol{X}}$ is not the Hermitian conjugate of $\boldsymbol{X}$; however, the determinant, Eq. (63), is real since $\boldsymbol{\Phi}\{\boldsymbol{A}\}$ is Hermitian. Indeed,

$$\boldsymbol{\Phi}\{\boldsymbol{A}\}=\begin{pmatrix}(\boldsymbol{TA})^{1/2} & \boldsymbol{0}\\ \boldsymbol{0} & (\boldsymbol{T}/\boldsymbol{A})^{1/2}\end{pmatrix}\begin{pmatrix}\boldsymbol{I} & \bar{\boldsymbol{X}}\\ \boldsymbol{X} & \boldsymbol{I}\end{pmatrix}\begin{pmatrix}(\boldsymbol{TA})^{1/2} & \boldsymbol{0}\\ \boldsymbol{0} & (\boldsymbol{T}/\boldsymbol{A})^{1/2}\end{pmatrix} = \begin{pmatrix}\boldsymbol{TA} & \boldsymbol{J}\\ \boldsymbol{J} & \boldsymbol{T}/\boldsymbol{A}\end{pmatrix}. \tag{64}$$

For example, for three layers,

$$\boldsymbol{X}=\begin{pmatrix}\dfrac{\delta\tau_1}{\bar{\tau}_1} & i\sqrt{\dfrac{\alpha_1}{\bar{\tau}_1\tau_2\alpha_2}} & -i\sqrt{\dfrac{\alpha_1}{\bar{\tau}_1\tau_3\alpha_3}}\\ -i\sqrt{\dfrac{\alpha_2}{\tau_2\bar{\tau}_1\alpha_1}} & 0 & i\sqrt{\dfrac{\alpha_2}{\tau_2\tau_3\alpha_3}}\\ i\sqrt{\dfrac{\alpha_3}{\tau_3\bar{\tau}_1\alpha_1}} & -i\sqrt{\dfrac{\alpha_3}{\tau_3\tau_2\alpha_2}} & 0\end{pmatrix}, \tag{65}$$

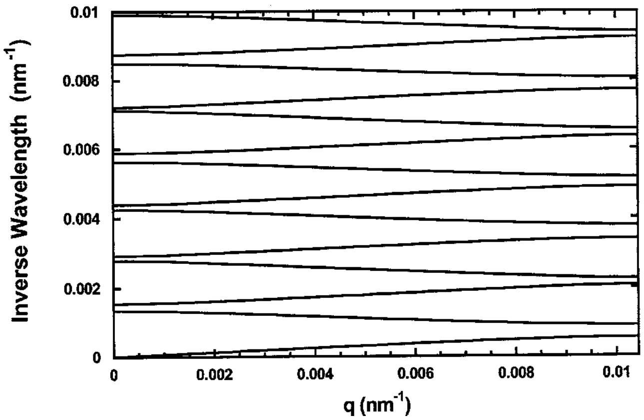

FIG. 8. The full band structure for the three-layer PBG of Fig. 1 as a function of wave vector q in the first Brillouin zone calculated with the use of Eq. (46).

and its determinant, $\|X\|=-\delta\tau_1/\bar{\tau}_1\tau_2\tau_3$ is real. As a function of A, $\bar{X}\{A\}=X\{A^{-1}\}$, and X and $\bar{X}$ are related by the similarity transformation $\bar{X}=A^{-1}XA$, so that they have the same eigenvalues ϑ; for example, for $\delta\tau_1=0$, they are given by

$$\vartheta = 0, \pm\left[\frac{1}{\tau_1\tau_3}+\frac{1}{\tau_3\tau_2}+\frac{1}{\tau_2\tau_1}\right]^{1/2}. \tag{66}$$

In the simplified notation, factoring out

$$\begin{pmatrix} (\boldsymbol{AT})^{1/2} & \mathbf{0}_N \\ \mathbf{0}_N & (\boldsymbol{TA}^{-1})^{1/2} \end{pmatrix} \tag{67}$$

on both sides of Eq. (40) leads to the Hermitian form

$$\boldsymbol{\Phi}(\boldsymbol{A})\begin{pmatrix} \boldsymbol{W}^+ \\ \boldsymbol{W}^- \end{pmatrix} = \begin{pmatrix} (\boldsymbol{AT})^{1/2} & \mathbf{0} \\ \mathbf{0} & (\boldsymbol{TA}^{-1})^{1/2} \end{pmatrix}\begin{pmatrix} \boldsymbol{I}_N & \bar{\boldsymbol{X}} \\ \boldsymbol{X} & \boldsymbol{I}_N \end{pmatrix} \times\begin{pmatrix} (\boldsymbol{AT})^{1/2}\boldsymbol{W}^+ \\ (\boldsymbol{TA}^{-1})^{1/2}\boldsymbol{W}^- \end{pmatrix} = 0, \tag{68}$$

where the meaning of the square roots, inverses, and the division of diagonal matrices $\boldsymbol{A}$ and $\boldsymbol{T}$ is clear.

Block diagonalization is achieved through multiplication,

$$\begin{pmatrix} \boldsymbol{I}_N & -\bar{\boldsymbol{X}} \\ -\boldsymbol{X} & \boldsymbol{I}_N \end{pmatrix}\begin{pmatrix} \boldsymbol{I}_N & \bar{\boldsymbol{X}} \\ \boldsymbol{X} & \boldsymbol{I}_N \end{pmatrix}\begin{pmatrix} (\boldsymbol{AT})^{1/2}\boldsymbol{W}^+ \\ (\boldsymbol{TA}^{-1})^{1/2}\boldsymbol{W}^- \end{pmatrix} = \begin{pmatrix} \boldsymbol{I}_N-\bar{\boldsymbol{X}}\boldsymbol{X} & \mathbf{0}_N \\ \mathbf{0}_N & \boldsymbol{I}_N-\boldsymbol{X}\bar{\boldsymbol{X}} \end{pmatrix}\begin{pmatrix} (\boldsymbol{AT})^{1/2}\boldsymbol{W}^+ \\ (\boldsymbol{TA}^{-1})^{1/2}\boldsymbol{W}^- \end{pmatrix} = \mathbf{0}. \tag{69}$$

In this form, (a) the two eigenvector problems are decoupled, (b) the eigenvalues are the same since from linear algebra,[30]

$$\|\boldsymbol{I}_N-\bar{\boldsymbol{X}}\boldsymbol{X}\| = \|\boldsymbol{I}_N-\boldsymbol{X}\bar{\boldsymbol{X}}\|, \tag{70}$$

(c) amplitudes $(\boldsymbol{TA}^{-1})^{1/2}\boldsymbol{W}^-$ are the eigenvectors of $\boldsymbol{I}_N-\boldsymbol{X}\bar{\boldsymbol{X}}$ and amplitudes $(\boldsymbol{AT})^{1/2}\boldsymbol{W}^+$ are the eigenvectors of $\boldsymbol{I}_N-\bar{\boldsymbol{X}}\boldsymbol{X}$, and (d) $\bar{\boldsymbol{X}}(\boldsymbol{TA}^{-1})^{1/2}\boldsymbol{W}^-$ is also an eigenvector $\boldsymbol{I}_N-\bar{\boldsymbol{X}}\boldsymbol{X}$ while $\boldsymbol{X}(\boldsymbol{AT})^{1/2}\boldsymbol{W}^+$ is also an eigenvector of $\boldsymbol{I}_N-\boldsymbol{X}\bar{\boldsymbol{X}}$.

B. Diagonalization of $X\bar{X}$

If $\boldsymbol{\Sigma}$ is the diagonal matrix with the eigenvalues σ_i of $\boldsymbol{X}\bar{\boldsymbol{X}}$ on the diagonals, then[28,29]

$$\|\boldsymbol{I}_N-\boldsymbol{X}\bar{\boldsymbol{X}}\| = \|\boldsymbol{I}_N-\boldsymbol{\Sigma}\| = \prod_{i=1}^{N}(1-\sigma_i), \tag{71}$$

which is real, so that σ_i are either real or occur in complex conjugate pairs. The eigenvalues can be found by evaluating the characteristic polynomial of $\boldsymbol{X}\bar{\boldsymbol{X}}$. Since $\boldsymbol{X}\bar{\boldsymbol{X}}$ is not Hermitian, the eigenvalues can be complex. Additional simplifications are possible at symmetry points since $\delta\tau_1=0$ and the matrix $\boldsymbol{J}$ is equal to i times a real skew-symmetric matrix, so that $\|\boldsymbol{J}\|=0$ and

$$\|\boldsymbol{X}\bar{\boldsymbol{X}}\| = 0. \tag{72}$$

Therefore, the constant term of the the characteristic polynomial

$$\|\boldsymbol{X}\bar{\boldsymbol{X}}-\sigma\| = (-\sigma)^N + \mathrm{tr}(\boldsymbol{X}\bar{\boldsymbol{X}})(-\sigma)^{N-1} + \cdots + \|\boldsymbol{X}\bar{\boldsymbol{X}}\| \tag{73}$$

is zero so that one of its solutions, $\sigma_N=0$, and the polynomial has $N-1$ generally nonzero σ_i eigenvalues $(i=1,\ldots,N-1)$. As a function of wavelength, eigenfrequencies correspond to $\sigma_i=1$ for some $i=1,\ldots,N-1$; the corresponding eigenvector can be used to calculate the wave amplitudes as demonstrated below. Therefore, eigenfrequencies can be labeled by the index $i=1,\ldots,N-1$ of the $\sigma_i=1$ eigenvalue. While analytic solutions are possible for low N, Eq. (71) is easily diagonalizable by computer for any N.

C. Demonstration for $N=3$

1. Characteristic polynomial

Using $\varsigma_i=\alpha_i\tau_i$ and $\xi_i=\tau_i/\alpha_i$, $\boldsymbol{X}$ is given by

$$\boldsymbol{X} = \begin{pmatrix} 0 & \frac{i}{\sqrt{\xi_1\zeta_2}} & -\frac{i}{\sqrt{\xi_1\zeta_3}} \\ -\frac{i}{\sqrt{\xi_2\zeta_1}} & 0 & \frac{i}{\sqrt{\xi_2\zeta_3}} \\ \frac{i}{\sqrt{\xi_3\zeta_1}} & -\frac{i}{\sqrt{\xi_3\zeta_2}} & 0 \end{pmatrix}, \tag{74}$$

and the matrix $\boldsymbol{X}\bar{\boldsymbol{X}}$ by

$$X\bar{X} = \begin{pmatrix} \frac{1}{\xi_1}\left(\frac{1}{\zeta_2}+\frac{1}{\zeta_3}\right) & -\frac{1}{\zeta_3}\sqrt{\frac{1}{\xi_1}\frac{1}{\xi_2}} & -\frac{1}{\zeta_2}\sqrt{\frac{1}{\xi_1}\frac{1}{\xi_3}} \\ -\frac{1}{\zeta_3}\sqrt{\frac{1}{\xi_1}\frac{1}{\xi_2}} & \frac{1}{\xi_2}\left(\frac{1}{\zeta_1}+\frac{1}{\zeta_3}\right) & -\frac{1}{\zeta_1}\sqrt{\frac{1}{\xi_2}\frac{1}{\xi_3}} \\ -\frac{1}{\zeta_2}\sqrt{\frac{1}{\xi_1}\frac{1}{\xi_3}} & -\frac{1}{\zeta_1}\sqrt{\frac{1}{\xi_2}\frac{1}{\xi_3}} & \frac{1}{\xi_3}\left(\frac{1}{\zeta_1}+\frac{1}{\zeta_2}\right) \end{pmatrix}. \tag{75}$$

The characteristic polynomial $\|X\bar{X}-\sigma\|$,

$$\|X\bar{X}-\sigma\| = -\sigma\left\{\sigma^2 - \left[\frac{1}{\xi_1}\left(\frac{1}{\zeta_2}+\frac{1}{\zeta_3}\right)+\frac{1}{\xi_2}\left(\frac{1}{\zeta_1}+\frac{1}{\zeta_3}\right) + \frac{1}{\xi_3}\left(\frac{1}{\zeta_1}+\frac{1}{\zeta_2}\right)\right]\sigma + \left[\frac{1}{\zeta_2}\frac{1}{\zeta_1}+\frac{1}{\zeta_2}\frac{1}{\zeta_3}+\frac{1}{\zeta_3}\frac{1}{\zeta_1}\right] \times\left[\frac{1}{\xi_1}\frac{1}{\xi_2}+\frac{1}{\xi_1}\frac{1}{\xi_3}+\frac{1}{\xi_2}\frac{1}{\xi_3}\right]\right\}, \tag{76}$$

contains no constant terms since $\|X\bar{X}\|=0$. (The coefficient of the quadratic term can be rewritten in a form symmetric in ζ,ξ.)

2. Eigenvalues and their classification

The eigenvalues of $X\bar{X}$ are the null eigenvalue $\sigma_3=0$ and two roots σ_1,σ_2 of the quadratic in the curly brackets of Eq. (76). It is convenient to relabel σ_1,σ_2 as $\sigma^{\pm}$ so that the determinant can be written as

$$\|\Phi\{A\}\| = \|T\|^2 \times \|I - X\bar{X}\| = [\|T\| \times (1-\sigma^+)] \times [\|T\| \times (1-\sigma^-)], \tag{77}$$

where based on the roots of Eq. (76) the two factors

$$\|T\| \times (1-\sigma^{\pm}) = \tau_1\tau_2\tau_3 - \left[\frac{\tau_1}{2}\left(\frac{\alpha_3}{\alpha_2}+\frac{\alpha_2}{\alpha_3}\right)+\frac{\tau_2}{2}\left(\frac{\alpha_1}{\alpha_3}+\frac{\alpha_3}{\alpha_1}\right) + \frac{\tau_3}{2}\left(\frac{\alpha_1}{\alpha_2}+\frac{\alpha_2}{\alpha_1}\right)\right] \pm \left\{\left[\frac{\tau_1}{2}\left(\frac{\alpha_3}{\alpha_2}+\frac{\alpha_2}{\alpha_3}\right) + \frac{\tau_2}{2}\left(\frac{\alpha_1}{\alpha_3}+\frac{\alpha_3}{\alpha_1}\right)+\frac{\tau_3}{2}\left(\frac{\alpha_1}{\alpha_2}+\frac{\alpha_2}{\alpha_1}\right)\right]^2 - (\alpha_1\tau_1 + \alpha_2\tau_2+\alpha_3\tau_3)\left(\frac{\tau_1}{\alpha_1}+\frac{\tau_2}{\alpha_2}+\frac{\tau_3}{\alpha_3}\right)\right\}^{1/2} = 0 \tag{78}$$

differ by the $\pm$ sign in front of the radical. The reverse process of multiplying $[\|T\|\times(1-\sigma^+)]\times[\|T\|\times(1-\sigma^-)]$ gives rise to Eq. (29), so that Eq. (78) is the sought factorization of the KP equation for $N=3$.

In the limit of $N=2$, $\tau_3=0$, and the condition $\|T\|\times(1-\sigma^{\pm})=0$ in Eq. (78) can be satisfied only when

$$[\alpha_1\tau_1+\alpha_2\tau_2]\left[\frac{\tau_1}{\alpha_1}+\frac{\tau_2}{\alpha_2}\right]=0, \tag{79}$$

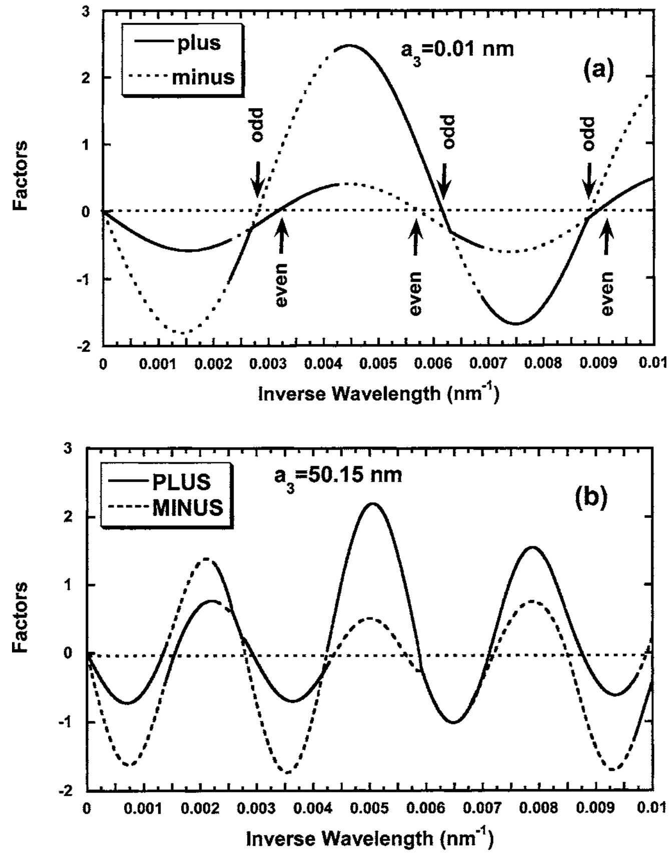

FIG. 9. The real parts of factors $\|T\|(1-\sigma^{\pm})$, Eq. (78), for a three-layer PBG (a_1=25.25 nm, a_2=75.2 nm, n_1=2.33, n_2=1.45, n_3=3.6) at $q=0$ as a function of inverse wavelength: (a) a_3 =0.01 nm (with parities noted) and (b) a_3=50.15 nm. The factors have been multiplied by $\cos(k_1a_1)\cos(k_2a_2)\cos(k_3a_3)$ in order to avoid singularities due to the tangents.

which is the factorization of the KP equation for $N=2$, Eq. (26), and provides the familiar conditions for odd- and even-parity states. In the limit of $N=2$ (here, using $a_3=0.01$ nm), Fig. 9(a) shows the plus and minus factors in Eq. (78) multiplied by $\cos(k_1a_1)\cos(k_2a_2)\cos(k_3a_3)$ in order to avoid singularities due to the tangents. The zeros of the two curves in Fig. 9(a) correctly identify the eigenfrequencies in Table I and the even-parity roots are bracketed by the odd-parity roots, as shown.

Next, in the vacuum limit $\alpha_i=1$, the curly brackets in Eq. (78) vanish identically, so that the remaining part of the expression $\|T\|(1-\sigma^{\pm})=\tau_1\tau_2\tau_3-\tau_1-\tau_2-\tau_3=0$ [see Eq. (30)] is the same for both roots and all the bands at $q=0,\pm\pi/d$ are doubly degenerate.

In general, the two eigenfrequency conditions $1-\sigma^{\pm}=0$ are satisfied at different wavelengths, except in the case of accidental degeneracies. Such degeneracies can be used to band gap engineer the structure to close some gaps. The real parts of the factors $\|T\|(1-\sigma^{\pm})$, Eq. (78), for the case of the PBG of Fig. 1 are plotted in Fig. 9(b), where the graphs have been multiplied by $\cos(k_1a_1)\cos(k_2a_2)\cos(k_3a_3)$ in order to avoid singularities due to the tangents. The zeros of the two factors occur exactly at the eigenfrequencies at $q=0$ in the band diagram in Fig. 8 or in the determinants plotted in Figs. 1 and 2. Each band can be labeled as $\pm$ depending on which of the two factors $\|\boldsymbol{T}\|(1-\sigma^{\pm})$ is zero. As in Fig. 9(a), the curves for $\|\boldsymbol{T}\|(1-\sigma^{+})$ and $\|\boldsymbol{T}\|(1-\sigma^{-})$ are separately discontinuous but each is the continuation of the other. The two curves merge whenever the imaginary parts are nonzero; along such segments, the eigenvalue condition $1-\sigma^{\pm}=0$ cannot be met. The discontinuities in Figs. 9(a) and 9(b) take place whenever $k_i a_i$ for one of the layers is an odd multiple of π—i.e., at the singularities of the respective tangents. Therefore, the $\pm$ label can change discontinuously along a band as a function of PBG dimensions (e.g., as in Fig. 5). Instead, eigenfrequencies can be classified according to whether the upper or lower curve passes through zero. This would provide a continous band label and is consistent with Fig. 9(a).

For $q=\pm\pi/d$, replace $\tau_1\to-1/\tau_1$ in this section.

3. Analytic wave functions

The wave functions corresponding to the $\sigma_i=1$ eigenvalue can be found analytically from the eigenvalue-eigenvector equation [see Eq. (69)],

$$(\boldsymbol{X}\bar{\boldsymbol{X}})\lfloor(\boldsymbol{T}\boldsymbol{A}^{-1})^{1/2}\boldsymbol{W}^{-}\rfloor=\sigma\lfloor(\boldsymbol{T}\boldsymbol{A}^{-1})^{1/2}\boldsymbol{W}^{-}\rfloor. \tag{80}$$

Defining $(\boldsymbol{T}\boldsymbol{A}^{-1})^{1/2}\boldsymbol{W}^{-}=\boldsymbol{V}$, the eigenvector equation to be solved is [see Eq. (75)]

$$\begin{pmatrix} \frac{1}{\xi_1}\left(\frac{1}{\varsigma_2}+\frac{1}{\varsigma_3}\right) & -\frac{1}{\varsigma_3}\sqrt{\frac{1}{\xi_1}\frac{1}{\xi_2}} & -\frac{1}{\varsigma_2}\sqrt{\frac{1}{\xi_1}\frac{1}{\xi_3}} \\ -\frac{1}{\varsigma_3}\sqrt{\frac{1}{\xi_1}\frac{1}{\xi_2}} & \frac{1}{\xi_2}\left(\frac{1}{\varsigma_1}+\frac{1}{\varsigma_3}\right) & -\frac{1}{\varsigma_1}\sqrt{\frac{1}{\xi_2}\frac{1}{\xi_3}} \\ -\frac{1}{\varsigma_2}\sqrt{\frac{1}{\xi_1}\frac{1}{\xi_3}} & -\frac{1}{\varsigma_1}\sqrt{\frac{1}{\xi_2}\frac{1}{\xi_3}} & \frac{1}{\xi_3}\left(\frac{1}{\varsigma_1}+\frac{1}{\varsigma_2}\right) \end{pmatrix}\begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix}=\begin{pmatrix} 1 \\ V_2 \\ V_3 \end{pmatrix}, \tag{81}$$

with the solution

$$\begin{pmatrix} W_1^- \\ W_2^- \\ W_3^- \end{pmatrix}=\begin{pmatrix} 1/\zeta_1\Psi_1 \\ 1/\zeta_2\Psi_2 \\ 1/\zeta_3\Psi_3 \end{pmatrix}, \tag{82}$$

where Ψ_i were defined in Eq. (52c). The other half of the eigenvector $\boldsymbol{W}$ is found from the relation $\boldsymbol{W}^{+}=-(\boldsymbol{T}\boldsymbol{A})^{-1}\boldsymbol{J}\boldsymbol{W}^{-}$, Eq. (58a), which ensures the proper phase relationship between the upper- and lower-amplitude components. Performing the indicated multiplications,

$$\boldsymbol{W}^{+}=-(\boldsymbol{T}\boldsymbol{A})^{-1}\boldsymbol{J}\boldsymbol{W}^{-}=-i\begin{pmatrix} 0 & \frac{1}{\zeta_1} & -\frac{1}{\zeta_1} \\ -\frac{1}{\zeta_2} & 0 & \frac{1}{\zeta_2} \\ \frac{1}{\zeta_3} & -\frac{1}{\zeta_3} & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{\zeta_1\Psi_1} \\ \frac{1}{\zeta_2\Psi_2} \\ \frac{1}{\zeta_3\Psi_3} \end{pmatrix}=-i\begin{pmatrix} \frac{1}{\zeta_1}\left(\frac{1}{\zeta_2\Psi_2}-\frac{1}{\zeta_3\Psi_3}\right) \\ \frac{1}{\zeta_2}\left(\frac{1}{\zeta_3\Psi_3}-\frac{1}{\zeta_1\Psi_1}\right) \\ \frac{1}{\zeta_3}\left(\frac{1}{\zeta_1\Psi_1}-\frac{1}{\zeta_2\Psi_2}\right) \end{pmatrix}. \tag{83}$$

Altogether, the amplitude coefficients for the three layers are

$$W_1=\frac{1}{\zeta_1}\begin{pmatrix} i\left(\frac{1}{\zeta_3\Psi_3}-\frac{1}{\zeta_2\Psi_2}\right) \\ \frac{1}{\Psi_1} \end{pmatrix}, W_2=\frac{1}{\zeta_2}\begin{pmatrix} i\left(\frac{1}{\zeta_1\Psi_1}-\frac{1}{\zeta_3\Psi_3}\right) \\ \frac{1}{\Psi_2} \end{pmatrix}, W_3=\frac{1}{\zeta_3}\begin{pmatrix} i\left(\frac{1}{\zeta_2\Psi_2}-\frac{1}{\zeta_1\Psi_1}\right) \\ \frac{1}{\Psi_3} \end{pmatrix}. \tag{84}$$

At $q=0$, the amplitudes of the traveling waves are found from Eq. (37a)

$$\boldsymbol{C}_i = \exp[-i\boldsymbol{K}_i(a_i + z_{i-1})]\sec(\boldsymbol{K}_i a_i)(\boldsymbol{M}_i^{-1}\boldsymbol{W}_i), \quad i = 1,2,3;$$

for example, for the first layer,

$$\boldsymbol{C}_1 = \begin{pmatrix} c_1^+ \\ c_1^- \end{pmatrix} = \frac{\sec(k_1 a_1)}{2\zeta_1}\begin{pmatrix} \exp(-ik_1a_1)\left[i\left(\frac{1}{\zeta_3\Psi_3} - \frac{1}{\zeta_2\Psi_2}\right) + \frac{1}{\alpha_1\Psi_1}\right] \\ \exp(ik_1a_1)\left[i\left(\frac{1}{\zeta_3\Psi_3} - \frac{1}{\zeta_2\Psi_2}\right) - \frac{1}{\alpha_1\Psi_1}\right] \end{pmatrix}, \tag{85}$$

and for other layers the results are found by the cyclic permutation of indices. Using the wave amplitudes from Eq. (85), the wave functions, Eq. (3),

$$\psi(z) = c_i^+ \exp(ik_i z) + c_i^- \exp(-ik_i z),$$

in the three layers are given, respectively, by the analytic expressions

$$\psi(z) = \begin{cases} \frac{\sec(k_1a_1)}{\zeta_1}\left[\left(\frac{1}{\zeta_3\Psi_3} - \frac{1}{\zeta_2\Psi_2}\right)\cos(k_1\zeta) + \frac{\tau_1}{\zeta_1\Psi_1}\sin(k_1\zeta)\right], & \zeta = z - a_1, \\ \frac{\sec(k_2a_2)}{\zeta_2}\left[\left(\frac{1}{\zeta_1\Psi_1} - \frac{1}{\zeta_3\Psi_3}\right)\cos(k_2\zeta) + \frac{\tau_2}{\zeta_2\Psi_2}\sin(k_2\zeta)\right], & \zeta = z - (2a_1 + a_2), \\ \frac{\sec(k_3a_3)}{\zeta_3}\left[\left(\frac{1}{\zeta_2\Psi_2} - \frac{1}{\zeta_1\Psi_1}\right)\cos(k_3\zeta) + \frac{\tau_3}{\zeta_3\Psi_3}\sin(k_3\zeta)\right], & \zeta = z - (2a_1 + 2a_2 + a_3), \end{cases} \tag{86}$$

where ζ is the distance to the middle of the respective layer. As a check, the continuity of the wave function, Eq. (86), at the interface between the first and second layers, $z=2a_1$, gives rise to the condition

$$\Psi_1\Psi_2\Psi_3 + \Psi_1\Psi_2 + \Psi_1\Psi_3 + \Psi_2\Psi_3 = 0$$

(and similarly for the other interfaces), which is precisely the eigenfrequency condition found earlier, Eq. (52b). The continuity of the weighted derivatives at interfaces leads to the identity $1=1$. Therefore, the wave functions in Eq. (86) solve the three layer problem.

The analytic expressions for the wave functions contain terms that are even and odd with respect to reflections across the centers of each layer. Therefore, it should be possible to design multilayers with controlled even and odd wave function content in order to exploit, for example, selection rules for a physical process of interest.

Overall, the case of $N=3$ demonstrates how the formalism can be used analytically to find eigenfrequencies and wave functions.

VIII. CONCLUSIONS

The eigenvalue-eigenvector problem for the frequency spectra and wave functions of arbitrary, one-dimensional, **N**-period layered systems have been formulated in terms of tangents only. The secular equation was shown to be a physical realization of the $2N\times 2N$ operator Riccati equation in the form of a $2N\times 2N$ Hermitian eigenvector-eigenvalue problem (main equation). The main equation was halved to a Hermitian $N\times N$ (submain) form, which made further analytic progress possible. The derived formalism is Hermitian, compact, algorithmically simple, and numerically stable. The eigenfrequency conditions can be represented by geometric figures such as a simple triangle or a tetrahedron for $N=3$. The analytic advantages of the present formalism were demonstrated by diagonalizing the submain equation for $N=3$ and deriving analytic eigenfrequency conditions and analytic wave functions for the three-layer problem. The diagonalization for any N makes it possible to classify eigenfrequencies according to the zeros of the eigenvalues of the submain equation. The analyticity of the formalism should facilitiate the band-gap engineering of the band structure and wave functions of multilayer structures. The ease of numerical implementation was demonstrated by calculating the frequency spectra and wave functions of a three-layer PBG. The present formalism can be applied to the calculation of the band spectra of any **N**-layer periodic system such as PBG stacks, the electronic structure of superlattices, and periodic phononic, plasmonic, polaronic, and magnetic structures.

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APPENDIX A

TABLE II. The notation and symbols used in the main text.

Symbol	Meaning	Symbol	Meaning
N	Number of layers	$\zeta_i=\tau_i\alpha_i$	Product, Eq. (47)
$2a_i$	Width of ith layer	$\boldsymbol{M}$	Matrix of materials parameters, Eq. (4)
d	Lattice period	$\boldsymbol{C},\boldsymbol{D},\boldsymbol{G},\boldsymbol{W}$	Column vectors of wave amplitudes, Eqs. (5), (13), (31), and (35)
λ	Wavelength in vacuum	$\boldsymbol{K}$	Matrix of wave numbers, Eq. (6)
n_i	Refractive index of ith layer	$\boldsymbol{\Lambda}$	Argument of matrix exponential, Eq. (10)
$k_i=2\pi n_i/\lambda$	Wave number	$\boldsymbol{A}_{ij}=\alpha_i\delta_{ij}$	Matrix of refractive indices, Eq. (42)
$\alpha_i=(n_i,n_i^{-1})$	TE-TM mode coefficient, Eq. (4)	$\boldsymbol{T}_{ij}=\tau_i\delta_{ij}$	Matrix of tangents, Eq. (41)
$\tau_i=tan\, k_ia_i$	Tangent for first layer	$\boldsymbol{J}$	Coupling matrix, Eq. (43)
q	Wave vector	$\boldsymbol{\Phi}$	Secular matrix, Eq. (40)
$\tau_1^{\pm}=tan(k_1a_1\pm qd/2)$	Tangents for ith layer, Eqs. (25a) and (25b)	$\boldsymbol{W}=\begin{pmatrix}\boldsymbol{W}^+\\ \boldsymbol{W}^-\end{pmatrix}$	Eigenvector of $\boldsymbol{\Phi}$, Eq. (40)
$\bar{\tau}_1=(\tau_1^-+\tau_1^+)/2$	Tangent average for first layer, Eqs. (25a) and (25b)	$\boldsymbol{X},\bar{\boldsymbol{X}}$	Auxiliary matrices, Eq. (61)
$\delta\tau_1=(\tau_1^--\tau_1^+)/2$	Tangent difference, Eqs. (25a) and (25b)	$\boldsymbol{U}$	Unitary transformation
$c_i=cos\, k_ia_i$ $s_i=sin\, k_ia_i$	Sines and cosines, Eq. (23)	$\boldsymbol{D}$	Diagonal matrix
$\xi_i=\tau_i/\alpha_i$	Ratio	$\boldsymbol{\Sigma},\boldsymbol{\sigma},\boldsymbol{\sigma}^{\pm}$	Eigenvalues, Eq. (71)

APPENDIX B: EXTENSION TO EVEN N

For even N, one may construct equations for $N+1$ (odd) and then set the $(N+1)$th tangent to zero. Alternately, for even N, Eq. (32) can be rearranged as follows[22]:

$$\begin{pmatrix} \tan(\boldsymbol{\Lambda}_1a_1-qd/2) & \tan\boldsymbol{\Lambda}_2a_2 & i\boldsymbol{I}_2 & \cdots & i\boldsymbol{I}_2 & -i\boldsymbol{I}_2 \\ -i\boldsymbol{I}_2 & \tan\boldsymbol{\Lambda}_2a_2 & \tan\boldsymbol{\Lambda}_3a_3 & \ddots & -i\boldsymbol{I}_2 & i\boldsymbol{I}_2 \\ i\boldsymbol{I}_2 & -i\boldsymbol{I}_2 & \tan\boldsymbol{\Lambda}_3a_3 & \ddots & \ddots & -i\boldsymbol{I}_2 \\ \vdots & \ddots & -i\boldsymbol{I}_2 & \ddots & \ddots & \vdots \\ i\boldsymbol{I}_2 & & \ddots & \ddots & \tan\boldsymbol{\Lambda}_{N-1}a_{N-1} & \tan\boldsymbol{\Lambda}_Na_N \\ \tan(\boldsymbol{\Lambda}_1a_1-qd/2) & i\boldsymbol{I}_2 & \cdots & \cdots & -i\boldsymbol{I}_2 & \tan\boldsymbol{\Lambda}_Na_N \end{pmatrix}\begin{pmatrix}\boldsymbol{W}_1\\ \boldsymbol{W}_2\\ .\\ .\\ \boldsymbol{W}_{N-1}\\ \boldsymbol{W}_N\end{pmatrix}=0, \tag{B1}$$

except that for $N=2$,

$$\begin{pmatrix} \tan(\boldsymbol{\Lambda}_1a_1-qd/2) & \tan\boldsymbol{\Lambda}_2a_2 \\ -i\boldsymbol{I}_2 & i\boldsymbol{I}_2 \end{pmatrix}\begin{pmatrix}\boldsymbol{W}_1\\ \boldsymbol{W}_2\end{pmatrix}=0, \tag{B2}$$

whose 2×2 secular determinant is [see Eq. (25b)]

$$\|\tan(\mathbf{\Lambda}_1 a_1 - qd/2) + \tan \mathbf{\Lambda}_2 a_2\| = \left\| \begin{matrix} \delta\tau_1 & \bar{\tau}_1/\alpha_1 + \tau_2/\alpha_2 \\ \alpha_1\bar{\tau}_1 + \alpha_2\tau_2 & \delta\tau_1 \end{matrix} \right\| = 0. \quad \text{(B3)}$$

For example, for $q=0$ and $\delta\tau_1=0$, $\boldsymbol{W}_1^{\pm}=\boldsymbol{W}_2^{\pm}$, and Eq. (B2) separates into two equations

$$(\alpha_1\tau_1 + \alpha_2\tau_2)\boldsymbol{W}_1^{+} = 0, \quad \text{odd parity}, \quad \text{(B4a)}$$

$$(\tau_1/\alpha_1 + \tau_2/\alpha_2)\boldsymbol{W}_1^{-} = 0, \quad \text{even parity}. \quad \text{(B4b)}$$

Manipulations of Eq. (B1), similar to those that led to the main equation, now give

$$\begin{pmatrix} \bar{\boldsymbol{T}}\boldsymbol{A} & \bar{\boldsymbol{J}} \\ \bar{\boldsymbol{J}} & \bar{\boldsymbol{T}}\boldsymbol{A}^{-1} \end{pmatrix} \begin{pmatrix} \boldsymbol{W}^{+} \\ \boldsymbol{W}^{-} \end{pmatrix} = \boldsymbol{0}, \quad \text{(B5)}$$

where all the block matrices are $N \times N$ and are defined as

$$\bar{\mathbf{T}} = \begin{pmatrix} \bar{\tau}_1 & \tau_2 & 0 & \cdots & 0 \\ 0 & \tau_2 & \tau_3 & \ddots & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & 0 & \tau_{N-1} & \tau_N \\ \bar{\tau}_1 & 0 & \cdots & 0 & \tau_N \end{pmatrix} \quad \text{(B6)}$$

and

$$\bar{\boldsymbol{J}} = \begin{pmatrix} \delta\tau_1 & 0 & i & \cdots & i & -i \\ -i & 0 & 0 & \ddots & -i & i \\ i & -i & 0 & \ddots & i & -i \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ i & -i & i & \cdots & 0 & 0 \\ \delta\tau_1 & i & -i & \cdots & -i & 0 \end{pmatrix}. \quad \text{(B7)}$$

Equation (B5) serves the same purpose for even N as Eq. (40) for odd N. It can also lead to a number of simplified expressions.

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$$(\boldsymbol{M}_i)^{-1} = \frac{1}{2}\begin{pmatrix} 1 & \alpha_i^{-1} \\ 1 & -\alpha_i^{-1} \end{pmatrix}.$$

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[27] E. L. Ivchenko and G. Pikus, *Superlattices and Other Heterostructures* (Springer-Verlag, New York, 1995).

[28] Fuzhen Zhang, *Matrix Theory* (Springer, New York, 1999); Thomas Kailath, *Linear Systems* (Prentice-Hall, Englewood Cliffs, NJ, 1980), p. 656. If $\boldsymbol{F}$ is invertible, then

$$\left\|\begin{matrix}\boldsymbol{F} & \boldsymbol{D}\\ \boldsymbol{C} & \boldsymbol{B}\end{matrix}\right\| = \|\boldsymbol{F}\| \times \|\boldsymbol{B}-\boldsymbol{C}\boldsymbol{F}^{-1}\boldsymbol{D}\|.$$

[29] Peter Lancaster and Miron Tismenetsky, *The Theory of Matrices*, 2nd ed. (Academic Press, New York, 1985).

[30] J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Clarendon, Oxford, 1965), p. 54, or observe that the forms below have the same determinants since

$$\begin{pmatrix}\boldsymbol{I} & \boldsymbol{0}\\ -\bar{\boldsymbol{X}} & \boldsymbol{I}\end{pmatrix}\begin{pmatrix}\boldsymbol{I} & \boldsymbol{X}\\ \bar{\boldsymbol{X}} & \boldsymbol{I}\end{pmatrix} = \begin{pmatrix}\boldsymbol{I} & \boldsymbol{X}\\ \boldsymbol{0} & \boldsymbol{I}-\bar{\boldsymbol{X}}\boldsymbol{X}\end{pmatrix},$$

$$\begin{pmatrix}\boldsymbol{I} & -\boldsymbol{X}\\ \boldsymbol{0} & \boldsymbol{I}\end{pmatrix}\begin{pmatrix}\boldsymbol{I} & \boldsymbol{X}\\ \bar{\boldsymbol{X}} & \boldsymbol{I}\end{pmatrix} = \begin{pmatrix}\boldsymbol{I}-\boldsymbol{X}\bar{\boldsymbol{X}} & \boldsymbol{0}\\ \bar{\boldsymbol{X}} & \boldsymbol{I}\end{pmatrix}.$$