

## New eigenvalue equation for the Kronig–Penney problem

Frank Szmulowicz

Citation: [American Journal of Physics](#) **65**, 1009 (1997); doi: 10.1119/1.18695

View online: <http://dx.doi.org/10.1119/1.18695>

View Table of Contents: <http://scitation.aip.org/content/aapt/journal/ajp/65/10?ver=pdfcov>

Published by the [American Association of Physics Teachers](#)

### Articles you may be interested in

[The Kronig–Penney model extended to arbitrary potentials via numerical matrix mechanics](#)

Am. J. Phys. **83**, 773 (2015); 10.1119/1.4923026

[Transport in the random Kronig–Penney model](#)

J. Math. Phys. **53**, 122109 (2012); 10.1063/1.4769219

[Elementary Excitations of Condensates in a Kronig–Penney Potential](#)

AIP Conf. Proc. **850**, 41 (2006); 10.1063/1.2354597

[Kronig–Penney model with the tail-cancellation method](#)

Am. J. Phys. **69**, 512 (2001); 10.1119/1.1326074

[Remarks about the manipulation of the Kronig–Penney model for the introduction into the energy band theory of crystals](#)

Am. J. Phys. **65**, 89 (1997); 10.1119/1.18571



American Association of **Physics Teachers**

Explore the **AAPT Career Center** –  
access hundreds of physics education and  
other STEM teaching jobs at two-year and  
four-year colleges and universities.

<http://jobs.aapt.org>



# New eigenvalue equation for the Kronig–Penney problem

Frank Szmulowicz

*Wright Laboratory, Materials Directorate, WL/MLPO, Wright–Patterson Air Force Base, Ohio 45433-7707*

(Received 3 February 1997; accepted 13 April 1997)

The Kronig–Penney equation (KPE) has long been used as a pedagogic tool for explaining the formation of energy bands in a periodic potential in the form of a one-dimensional periodic array of square wells. However, the KPE does not readily reduce to the solution for an isolated square well in the limit of a large well-to-well separation. Moreover, the solutions at the center and the edge of the Brillouin zone are also not readily obtainable from the KPE. Computationally, the KPE can be inconvenient as it can vary over tens of orders of magnitude as the energy is increased from the bottom to the top of the well. In this paper, a new technique is developed for solving the Kronig–Penney problem and an alternative to the KPE is developed. The new eigenvalue equation has the conceptual advantage of immediately reducing to the equation for an isolated square well in the limit of infinite barrier width and of immediately providing the equation for the top and bottom of a band as well as the computational advantage of being on the order of unity. © 1997 American Association of Physics Teachers.

## I. INTRODUCTION

The Kronig–Penney (KP) model<sup>1</sup> provides the solution for the energy band structure of an electron in a periodic array of square wells separated by finite-width barriers. In the past half-century, the KP problem has become a standard topic in

most quantum mechanics<sup>2,3</sup> and solid state textbooks<sup>4,5</sup> because of its fundamental importance to the development of quantum mechanics and solid state theory. Recently, as the result of progress in microfabrication and nanolithography, the model has been found to be applicable to a number of

problems involving artificially structured materials, in particular, semiconductor superlattices.<sup>6,7</sup> In the latter case, the KP model is the simplest manifestation of a very sophisticated envelope-function approach for the calculation of the energy spectra of electrons and holes.<sup>6-8</sup> Among many of its applications, the model has been used in the case of two-dimensional electrons moving in a one-dimensional periodic magnetic field<sup>9</sup> and of photons moving between two facing gratings or in a medium with a periodically varying refractive index.<sup>10</sup> To derive the KP equation (KPE), one must evaluate a  $4 \times 4$  determinant, a tedious process at best.<sup>4</sup> Surprisingly, from the conceptual and pedagogic points of view, the resulting solution does not appear to readily reduce to the solution for an isolated square well in the limit of infinite well separation. Moreover, the conditions for the top and bottom of an energy band are best obtained not from the KPE itself but from redoing the problem with wave functions symmetric and antisymmetric about the centers of the wells and barriers.<sup>7</sup> Last, for typical periodic potential parameters and energies below the top of the barrier, the KPE can vary over tens of orders of magnitude, which can become computationally inconvenient.<sup>3</sup> A number of issues in the numerical handling of the KPE can be found in the work of Lippmann.<sup>11</sup> In this paper, these problems are addressed by deriving an alternative equation for the KP model. At the same time, an original technique for solving the KP problem is developed.

## II. STANDARD SOLUTION TO THE KRONIG-PENNEY PROBLEM

### A. Schrödinger equation for the Kronig-Penney problem

Figure 1 shows the potential experienced by an electron in a one-dimensional array of square wells along the  $z$  direction. The Schrödinger equation for an electron in the potential of Fig. 1 is<sup>1-7</sup>

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(z)}{dz^2} + V(z)\Psi(z) = E\Psi(z), \quad (1)$$

where  $m$  is the electron mass,  $\Psi$  is the wave function,  $E$  is the energy, and  $V(z) = V(z+d)$  is the periodic one-dimensional potential, where  $d$  is the period. It is well known that the solutions of Eq. (1) must obey the Bloch periodicity condition<sup>1-7</sup>

$$\Psi(z+d) = e^{iqd}\Psi(z), \quad (2)$$

where  $-\pi/d < q \leq \pi/d$  is the wave vector spanning the one-dimensional Brillouin zone. As a result, the  $q$  vector labels

the eigenstates of Eq. (1), and the energy eigenvalues  $E = E(q)$  are a function of  $q$ . The KP problem consists of solving Eq. (1) for the energies and wave functions of electrons in the potential of Fig. 1.

### B. Square-well limit

One of the goals of this paper is to show an isolated square-well limit of the energy eigenvalue equation for the periodic array of square wells. For completeness sake then, consider the eigenvalue equation for a single, isolated square well of width  $2b$  and height  $V$  for a carrier of mass  $m$ . The well-known solution for  $E < V$ , obtained by requiring the continuity of the wave function  $\Psi$  and its derivative  $\Psi'$  at one boundary, say  $z = b$ , is given by<sup>2-7</sup>

$$\tan k_B b = \beta \quad \text{for even parity levels}, \quad (3)$$

$$\tan k_B b = -\beta^{-1} \quad \text{for odd parity levels}, \quad (4)$$

where  $\beta \equiv \kappa_A/k_B$ ,  $k_A = \sqrt{2m(E-V)/\hbar^2} \equiv i\kappa_A$ , and  $k_B = \sqrt{2mE/\hbar^2}$ . Equations (3) and (4) will be used later for comparison with the KPE. In the case of the KPE, it will be apparent that its form is not readily reducible to that of Eqs. (3) and (4) as the barrier width  $a \rightarrow \infty$ .

### C. Boundary conditions and the Kronig-Penney equation

To obtain the eigenvalue equation for the KP problem, one must first set up the boundary conditions for the wave function which satisfies the Schrödinger equation, Eq. (1), in the well and barrier regions. Let the periodic potential consist of an infinite succession of materials  $A$  of width  $2a$  (barrier) and material  $B$  of width  $2b$  (well), with period  $d = 2a + 2b$ . Because of the Bloch periodicity condition, it is necessary to solve Eq. (1) in only one period of the potential, say the zeroth period,  $-b \leq z < b + 2a$ . The wave function in the zeroth period is a sum of plane waves propagating in the positive and negative directions,<sup>1-7</sup>

$$\Psi(z) = \begin{cases} c_1^A e^{ik_A z} + c_2^A e^{-ik_A z}, & b \leq z < b + 2a \\ c_1^B e^{ik_B z} + c_2^B e^{-ik_B z}, & -b \leq z < b \end{cases}. \quad (5)$$

The boundary conditions on the wave function and its derivative at two interfaces,  $z = \pm b$ , supplemented by the Bloch periodicity condition, Eq. (2), give rise to a secular equation, implicit in energy, for the eigenvalues and eigenfunctions,<sup>3,4</sup>

$$\begin{pmatrix} e^{ik_A b} & e^{-ik_A b} & -e^{ik_B b} & -e^{-ik_B b} \\ k_A e^{ik_A b} & -k_A e^{-ik_A b} & -k_B e^{ik_B b} & k_B e^{-ik_B b} \\ e^{ik_A(d-b)-qd} & e^{-ik_A(d-b)-qd} & -e^{-ik_B b} & -e^{ik_B b} \\ k_A e^{ik_A(d-b)-qd} & -k_A e^{-ik_A(d-b)-qd} & -k_B e^{-ik_B b} & k_B e^{ik_B b} \end{pmatrix} \begin{pmatrix} c_1^A \\ c_2^A \\ c_1^B \\ c_2^B \end{pmatrix} = 0. \quad (6)$$

The first/second row gives the continuity of the wave function and its derivative, respectively, at  $z=b$ ; the third/fourth row gives the continuity of the wave function and its derivative, respectively, at  $z=-b$ .

For a nontrivial solution of Eq. (6), the determinant of the matrix in Eq. (6) must be zero. After a tedious calculation of the determinant, one obtains the well-known KPE:<sup>1-7</sup>

$$\cos qd = \cos 2k_B b \cos 2k_A a - \frac{1}{2}(\alpha + 1/\alpha) \sin 2k_B b \sin 2k_A a, \quad (7a)$$

where<sup>1-7</sup>  $\alpha = k_A/k_B$ ; also, for energies below the top of the barrier,  $E < V$ , Eq. 7(a) becomes<sup>1-7</sup>

$$\cos qd = \cos 2k_B b \cosh 2\kappa_A a + \frac{1}{2}(\beta - 1/\beta) \sin 2k_B b \sinh 2\kappa_A a. \quad (7b)$$

The solution for the associated eigenvector from the matrix equation, Eq. (6), is also tedious to find.

### D. Critique of the Kronig–Penney equation

The KPE contains a wealth of information on the energy bands for a periodic array of square wells. However, even though the potential has the form of square wells separated by barriers, the forms of Eq. (7b) and Eqs. (3) and (4) have very little in common. For that reason, it takes about eight additional, nonintuitive steps to reduce Eq. (7b) to Eqs. (3) and (4) in the limit of infinite barrier width.

In addition, the solutions of Eqs. (7a) and (7b) at the center,  $q=0$ , and the edges,  $q = \pm \pi/d$ , of the Brillouin zone [see Eqs. (22) and (23)] are not readily apparent. In fact, these solutions are best found by starting the problem over, constructing wave functions which are even and odd with respect to the centers of wells and barriers, setting up the requisite boundary conditions, and solving the resulting determinantal equations again.<sup>12</sup>

As important, Eq. (7b) is computationally inconvenient, as the following example demonstrates. Let the potential parameters be given by well depth  $V=0.3$  eV, well width  $2b=200$  Å, and barrier width  $2a=500$  Å, which is typical of modern-day semiconductor superlattices fabricated by molecular beam epitaxy.<sup>6,7</sup> For these parameters (and using the free electron mass), the hyperbolic sines and cosines are on the order of  $10^{60}$  for the energy at the bottom of the well and on the order of unity for the energy at the top of the well. As a result, in this energy range, Eq. (7b) oscillates over 60 orders of magnitude. These wide oscillations are inconvenient when using a hand-held calculator or even when searching for the roots of Eq. (7b) on a mainframe.

The alternative to the KPE provided in this paper, Eqs. (20a) and (20b) is free of these three problems.

## III. ALTERNATIVE EQUATION

### A. Notational simplification

In order to derive an alternative to the KPE, a new technique for solving Eq. (6) is developed here. The initial improvement is merely notational, yet it later allows greater freedom in manipulating the secular matrix. The technique exhibited below should be within the capabilities of most students advanced enough to study the Kronig–Penney prob-

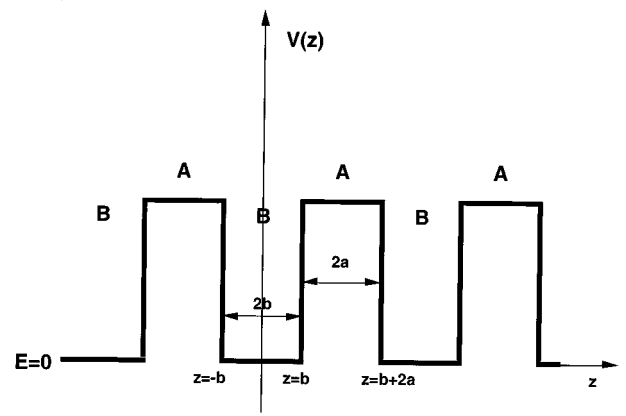


Fig. 1. The one-dimensional potential profile for a periodic array of square wells. Letters A and B denote the barrier and well regions, respectively. The zero of energy is chosen at the bottom of the well; the barriers have height  $V$ .

lem. Those not familiar with the manipulations below should still appreciate the result contained in Eqs. (19) and (20a) and (20b).

Since all the dimensional information is contained in the exponential factors, it is possible to separate the dimensional and material properties by writing Eq. (6) succinctly in the following form:

$$\begin{pmatrix} M_A \exp(iK_A b) & -M_B \exp(iK_B b) \\ e^{-iqd} M_A \exp(iK_A(d-b)) & -M_B \exp(-iK_B b) \end{pmatrix} \times \begin{pmatrix} C^A \\ C^B \end{pmatrix} = 0, \quad (8)$$

where the upper/lower rows give the boundary conditions at  $z=b, -b$ , respectively. Various terms in Eq. (8) are defined as follows:

$$M_A = \begin{pmatrix} 1 & 1 \\ k_A & -k_A \end{pmatrix}, \quad C^A = \begin{pmatrix} c_1^A \\ c_2^A \end{pmatrix}, \quad K_A = \begin{pmatrix} k_A & 0 \\ 0 & -k_A \end{pmatrix}, \quad (9)$$

and similarly for quantities with subscript  $B$ . For future reference, the matrix inverse of  $M_A$  is

$$M_A^{-1} = \frac{1}{2} \begin{pmatrix} 1 & 1/k_A \\ 1 & -1/k_A \end{pmatrix}. \quad (10)$$

As usual, the exponential of a matrix is defined in terms of the series expansion<sup>13</sup>

$$e^N = I + N + N^2/2! + N^3/3! + \dots, \quad (11)$$

where  $I$  is the identity matrix. Here, since  $K_A$  is diagonal, all functions of  $K_A$  are diagonal as well; in particular,

$$\exp(iK_A b) = \begin{pmatrix} \exp(ik_A b) & 0 \\ 0 & \exp(-ik_A b) \end{pmatrix}. \quad (12)$$

Therefore, the validity of Eq. (8) derives, in part, from the validity of Eq. (12). The ultimate proof of the validity of Eq.

(8) is the fact that when Eq. (8) is multiplied out, one obtains Eq. (6). Because of these notational simplifications, it will be possible to manipulate Eq. (8) further and to obtain new results later on in this paper.

## B. Reduction to tangents-only form

Since Eqs. (3) and (4) contain tangents, the goal here is to use Eq. (8) to obtain an eigenvalue equation in terms of tangents alone. To produce such an alternative form, one must first replace exponentials in Eq. (8) by trigonometric functions.

Using simple row addition, subtraction, and factoring (see the hints in the Appendix), Eq. (8) can be transformed into

$$\begin{pmatrix} I & -M_B \cos K_B b \\ M_B \tan(K_B b) M_B^{-1} + M_A \tan(K_A a - qd/2) M_A^{-1} & 0 \end{pmatrix} \begin{pmatrix} X \\ C^B \end{pmatrix} = 0, \quad (14)$$

where

$$X = \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix} \equiv M_A \cos(K_A a - qd/2) \times \exp(i(K_A - qI)d/2) C^A; \quad (15)$$

also, from the first row of Eq. (14), we have

$$X = M_B \cos(K_B b) C^B. \quad (16)$$

Except when one of the cosine matrices is not invertible (i.e., whenever the determinants  $\|\cos(K_B b)\| = 0$  or  $\|\cos(K_A a - qd/2)\| = 0$  at points of measure zero), the second row of Eq. (14) furnishes the following linear equation of order  $2 \times 2$ :

$$(M_B \tan(K_B b) M_B^{-1} + M_A \tan(K_A a - qd/2) M_A^{-1}) X = 0. \quad (17)$$

For a nontrivial solution to exist, the determinant of the matrix in Eq. (17) must be zero, resulting in a novel secular equation given by

$$\|M_B \tan(K_B b) M_B^{-1} + M_A \tan(K_A a - qd/2) M_A^{-1}\| = 0. \quad (18)$$

The zeros of Eq. (18) as a function of energy furnish the energy eigenvalues for the periodic array of square wells. Once the zeroes of Eq. (18) are found, eigenvector  $X$  is found from Eq. (17), and then  $C^A$  and  $C^B$  are found from Eqs. (15) and (16), respectively. Because Eq. (17) is of order  $2 \times 2$ , the eigenvector is found more easily than from the original  $4 \times 4$  equation, Eq. (6).

Equation (18) accomplishes the goal of producing the sought-after tangents-only form but, to be useful, one must insert the definitions of the relevant matrices, which is done next.

## C. Alternative secular equation

Inserting the matrix definitions from Eqs. (9) and (10) into Eq. (17) results in the following  $2 \times 2$  equation:

$$\begin{pmatrix} M_A \cos(K_A a - qd/2) & -M_B \cos K_B b \\ M_A \sin(K_A a - qd/2) & M_B \sin K_B b \end{pmatrix} \times \begin{pmatrix} \exp(i(K_A - qI)d/2) C^A \\ C^B \end{pmatrix} = 0. \quad (13)$$

As with exponentials of a matrix, Eq. (12), the trigonometric functions of a matrix are defined in terms of their series expansions, and in the present case are diagonal matrices themselves.

Next, the lower-right element of the matrix is annihilated by adding an appropriate multiple of the first row to the second row (see the hints in the Appendix), yielding

$$\begin{pmatrix} \frac{A^- - A^+}{2} & \frac{1}{k_A} \left( \frac{A^- + A^+}{2} \right) + \frac{B}{k_B} \\ k_A \left( \frac{A^- + A^+}{2} \right) + k_B B & \frac{A^- - A^+}{2} \end{pmatrix} \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix} = 0, \quad (19)$$

where  $A^\pm = \tan(k_A a \pm qd/2)$  and  $B = \tan k_B b$ . The determinant of Eq. (19) furnishes the alternative secular equation

$$(A^+ + \alpha B)(A^- + B/\alpha) + (A^- + \alpha B)(A^+ + B/\alpha) = 0; \quad (20a)$$

using the symmetry  $(A, a) \leftrightarrow (B, b)$ , Eq. (20a) is equivalent to

$$(B^+ + \alpha A)(B^- + A/\alpha) + (B^- + \alpha A)(B^+ + A/\alpha) = 0; \quad (20b)$$

where  $B^\pm = \tan(k_B b \pm qd/2)$  and  $A = \tan k_A a$ . One attraction of the present technique is that a number of additional equivalent forms to Eqs. (20a) and (20b) can be derived starting with Eq. (8).

Equations (20a) and (20b) contain tangents only and, together with Eq. (19), represent the central result of this paper.

## D. Properties of the alternative secular equation

The present eigenvalue equation can be shown by trigonometric identities to be equivalent to the standard KPE; therefore, it yields the same solutions as the KPE. [Hint: multiply Eq. (20a) by  $\cos(k_A a + qd/2) \cos(k_A a - qd/2) \cos^2 k_B b$  and use double angle identities. However, the reverse proof of going from the KPE to the present Eq. (20), without the benefit of the forward proof, is not at all obvious.] Just as the original KPE, Eqs. (20) are even in  $q$ , because  $A^+ \leftrightarrow A^-$  as  $q \rightarrow -q$ , so that  $E(-q) = E(q)$ , and can be shown to be invariant under the interchange  $(A, a) \leftrightarrow (B, b)$ . These properties are best seen by using Eq. (20a) to derive the following identity:

$$(A + \alpha B)(A + B/\alpha) - (1 - \alpha AB)(1 - AB/\alpha)(\tan^2 qd/2) = 0, \quad (21)$$

which also makes it apparent that the equation is always real. Also, because of the periodicity of the squared tangent in Eq.

(21), the energy bands are periodic with the period  $2\pi/d$  of the Brillouin zone.

The tangents-only form of Eqs. (20a) and (20b) makes the present solution more akin to the underlying square-well problem, Eqs. (3) and (4). Another immediate benefit of Eq. (20) is that it is simple to obtain the conditions for the band extrema at  $q=0, \pm\pi/d$ , conditions which are not immediately apparent in the standard KPE.<sup>12</sup> However, in the present formalism, Eqs. (20a) and (20b) [or Eq. (21)] immediately yield for even parity bands

$$q=0, \quad \tan k_B b = \begin{cases} \beta \tanh \kappa_A a & \xrightarrow{a \rightarrow \infty} \beta \\ -\alpha \tan k_A a \end{cases}, \quad (22)$$

$$q = \pm \pi/d,$$

$$\tan k_B b = \begin{cases} \beta \coth \kappa_A a & \xrightarrow{a \rightarrow \infty} \beta \\ \alpha \cot k_A a \end{cases},$$

and for odd parity bands,

$$q=0, \quad \tan k_B b = \begin{cases} -\tanh \kappa_A a / \beta & \xrightarrow{a \rightarrow \infty} -1/\beta \\ -\tan k_A a / \alpha \end{cases}, \quad (23)$$

$$q = \pm \pi/d,$$

$$\tan k_B b = \begin{cases} -\coth \kappa_A a / \beta & \xrightarrow{a \rightarrow \infty} -1/\beta \\ \cot k_A a / \alpha \end{cases},$$

where even and odd refer to the parity of the associated wave functions about the centers of the wells and barriers and the upper/lower lines are for energies below/above the top of the well, respectively.

Clearly, in the limit of infinite barriers,  $a \rightarrow \infty$ , one recovers the conditions for the even and odd parity bound levels of an isolated square well, Eqs. (3) and (4). Moreover, Eqs. (20) have this property for any  $q$ . [This is best seen by letting  $a \rightarrow \infty$  in Eq. (24) below.]

At a general  $q$ , one can solve Eq. (20a) and obtain the heretofore unknown form for  $B$ ,

$$B = -\frac{\eta(A^- + A^+)}{4} \left[ 1 \pm \sqrt{1 - \left[ \frac{4}{\eta(A^- + A^+)} \right]^2 A^+ A^-} \right], \quad (24)$$

where  $\eta = \alpha + 1/\alpha$ . Because  $k_B = \sqrt{2mE/\hbar^2}$ , Eq. (24) can be used to formally obtain an expression for energy. At the middle of a band,  $q = \pm\pi/2d$ , Eq. (24) simplifies to

$$\tan k_B b = -\frac{\eta \tan 2k_A a}{2} \left[ 1 \pm \sqrt{1 + \left( \frac{2}{\eta} \cot 2k_A a \right)^2} \right], \quad (25)$$

a formerly unavailable analytic form.

As important, the present formalism is computationally more convenient. For example, for states below the top of the barrier at  $q=0$ , Eqs. (20a) and (20b) become

$$D = [\tan(k_B b) + \tanh(\kappa_A a)/\beta][\tan(k_B b) - \beta \tanh(\kappa_A a)] = 0, \quad (26)$$

where the two factors correspond to the odd and even parity solutions. To remove the possible singularities due to the tangents, it is better examine  $D \cos^2(k_B b)$ . Because hyperbolic tangents are bounded by  $\pm 1$ , the resulting expression is on the order of unity regardless of the barrier width  $a$ , proving the point about the numerical convenience. The same is true of Eqs. (20) for a general  $q$ . As a result, one can plot Eqs. (20) or (26) on a hand-held calculator in class or more easily find its roots even on a mainframe.

Although not demonstrated in this paper, one can easily find the eigenvector in Eq. (19), especially at  $q=0$  and  $\pm\pi/d$ , for which the diagonals are zero and the eigenvectors are  $X = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ ; using Eqs. (15) and (16), the resulting wave functions in Eq. (5) are eigenstates of parity.

## IV. SUMMARY

In conclusion, a new tangents-only form of the KP equation for a periodic array of square wells was developed. Its form is closely related to the underlying square-well problem as it can be immediately reduced to the solutions for an isolated square well in the limit of infinite barriers; also, it can be immediately used to provide the conditions for the top and bottom of a band, besides being useful at general wave vectors  $q$  for calculations of eigenenergies and wave functions. Moreover, for states below the top of the barrier, the present eigenvalue equation is more computationally convenient, being on the order of unity, whereas the Kronig-Penney equation varies over many orders of magnitude for a typical example. The solution technique demonstrated here can be used to extract other useful identities (e.g., for a delta-function periodic potential), besides being applicable to other one-dimensional periodic problems, such as elastic, magnetic, and optical periodic media. Therefore, from the conceptual, pedagogic, and practical point of view, the present approach should profitably supplement the standard Kronig-Penney treatment.

## APPENDIX

### 1. Steps leading to Eq. (13)

*Step 1:* Use Eq. (8). Factor out  $\exp i(K_A - qI)d/2$  (on the right-hand side) from column 1 and combine this factor with  $C^A$ :

$$\begin{pmatrix} M_A \exp i(-K_A a + qdI/2) & -M_B \exp(iK_B b) \\ M_A \exp i(K_A a - qdI/2) & -M_B \exp(-iK_B b) \end{pmatrix} \times \begin{pmatrix} e^{i(K_A - qI)d/2} C^A \\ C^B \end{pmatrix} = 0.$$

*Step 2:* Recall that  $(e^{iN} + e^{-iN})/2 = \cos N$  and  $(e^{iN} - e^{-iN})/2i = \sin N$ , in the sense of Eq. (11). Now add row 1

to row 2 and then divide by two; use this as new row 1. Then subtract row 1 from row 2 and divide the result by  $2i$ ; use the resulting equation as the new row 2:

$$\begin{pmatrix} M_A \cos(K_A a - qdI/2) & -M_B \cos(K_B b) \\ M_A \sin(K_A a - qdI/2) & M_B \sin(K_B b) \end{pmatrix} \times \begin{pmatrix} e^{i(K_A - qI)d/2} C^A \\ C^B \end{pmatrix} = 0. \quad (13)$$

Other ways of factoring the  $q$ -dependent exponential will lead to equivalent forms, for example, Eq. (20b).

## 2. Steps leading to Eq. (14)

Step 1: Multiply row 1 of Eq. (13) on the left by

$$\begin{aligned} (M_B \sin K_B b)(M_B \cos K_B b)^{-1} \\ = M_B \sin K_B b (\cos K_B b)^{-1} M_B^{-1} \\ = M_B (\tan K_B b) M_B^{-1}, \end{aligned}$$

where all the factors are understood to be matrices. The multiplication makes the “12” element into the additive inverse of the “22” element. Adding the result to row 2 makes the “22” element equal to zero. Use the result as new row 2, but keep row 1 unchanged:

$$\begin{pmatrix} M_A \cos(K_A a - qdI/2) & -M_B \cos(K_B b) \\ [M_B \tan(K_B b) M_B^{-1}] M_A \cos(K_A a - qdI/2) & 0 \\ + M_A \sin(K_A a - qdI/2) & \end{pmatrix} \begin{pmatrix} e^{i(K_A - qI)d/2} C^A \\ C^B \end{pmatrix} = 0.$$

Now factor out  $M_A \cos(K_A a - qdI/2)$  on the right from column 1 and combine it with the upper element of the eigenvector, which results in

$$\begin{pmatrix} I & -M_B \cos K_B b \\ M_B \tan(K_B b) M_B^{-1} + M_A \tan(K_A a - qdI/2) M_A^{-1} & 0 \end{pmatrix} \begin{pmatrix} X \\ C^B \end{pmatrix} = 0. \quad (14)$$

<sup>1</sup>R. L. de Kronig and W. G. Penney, “Quantum mechanics of electrons in crystal lattices,” *Proc. R. Soc. London, Ser. A* **130**, 499–513 (1931).

<sup>2</sup>Eugen Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970), 2nd ed., pp. 100–105.

<sup>3</sup>Robert B. Leighton, *Principles of Modern Physics* (McGraw-Hill, New York, 1959), pp. 396–400.

<sup>4</sup>C. Kittel, *Introduction to Solid State Physics* (Wiley, New York, 1976), 5th ed., pp. 191–192.

<sup>5</sup>N. W. Ashcroft and N. David Mermin, *Solid State Physics* (Holt, New York, 1976), pp. 146–149.

<sup>6</sup>G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures* (Wiley, New York, 1988), pp. 18–26.

<sup>7</sup>G. Bastard, J. A. Brum, and R. Ferreira, in *Solid State Physics: Semiconductor Heterostructures, and Nanostructures*, edited by H. Ehrenreich and D. Turnbull, *Solid State Physics*, Vol. 44 (Academic, New York, 1991),

pp. 250–284.

<sup>8</sup>F. Szmulowicz, “Numerically stable Hermitian secular equation for the envelope-function approximation for superlattices,” *Phys. Rev. B* **54**, 11 539–11547 (1996), and references therein.

<sup>9</sup>I. S. Ibrahim and F. M. Peeters, “The magnetic Kronig–Penney model,” *Am. J. Phys.* **63**, 171–174, and references therein.

<sup>10</sup>K. Todor and S. Hayese, “Formation of pseudo one-dimensional photonic band in visible region by grating pair method,” *Appl. Phys. Lett.* **70**, 550–552 (1997).

<sup>11</sup>H. Lippmann, “Remarks about the manipulation of the Kronig–Penney model for the introduction into the energy band theory of crystals,” *Am. J. Phys.* **65**, 89–92 (1997), and references therein.

<sup>12</sup>See Ref. 7, pp. 265–266.

<sup>13</sup>See, for example, Ref. 2, p. 167.

### DEPTH & MAJESTY OF FLOW

...HENRY lectures to the Juniors again this morning & I again attend. His manner grows more & more interesting, every time he lectures. He grows upon you. There's no popping up & then popping out about him. He isn't a kind of Water Pot that thro' a number of small holes allows his Instructions to filter through & drizzle out on the Understandings of his Pupils—but he is a Great Canal—laugh not at the Simile—like a Canal in its Constancy Uniformity, Depth & Majesty of Flow. Or like his own *Galvanism*—a Strong & Constant & Powerful Current—not possessing the momentary pungency & the Rapid Brilliancy of *Electricity* is true, but having that which it has not, a Continuity & a Deep Power in it that lasts & lasts with strong *Effect*...

Excerpt from the Diary of John R. Buhler, Princeton University (1846), in *The Papers of Joseph Henry*, edited by Marc Rothenberg (Smithsonian Institution Press, Washington, 1992), Vol. 6, p. 430.