Tight-Binding Analysis of Coupled Dielectric Waveguide Structures

P. Khalili Amiri
pkhalili@ee.sharif.edu

S. Fathololoumi
saeedf@ee.sharif.edu

M. Ranjbaran
ranjbaran@mehr.sharif.edu

K. Mehrany
mehrany@mehr.sharif.edu

B. Rashidian
rashidia@sina.sharif.edu

Department of Electrical Engineering, Sharif University of Technology, Tehran, Iran.

Abstract: Based on the mathematical similarity of the Schrödinger and Helmholtz equations, the tight-binding method has been employed for solving optical waveguide problems, in a manner similar to the methods commonly used in solid state physics. The solutions (TE mode waveforms and propagation constants) of a single dielectric waveguide are considered to be known, and tight-binding is used to compute the propagation constants of several multi-waveguide structures. Analytical solutions are derived for linear and circular arrays of adjacent waveguides. The problem of two similar adjacent waveguides is treated in detail with the propagation modes of the waveguides being similar or different. For this case, computer simulation is used to compare the proposed method to BPM (Beam Propagation Method) to test its validity. The results of the two approaches agree satisfactorily. Three examples further illustrate the proposed method and clarify the effect of defects in the waveguide array on the obtained band diagram.

Keywords: Tight-Binding, Dielectric Waveguide, Coupling, Photonic Bandgap, Beam Propagation Method.

1 Introduction

Dielectric waveguides are a vital part of integrated optical systems. Although their basic operation may be partly understood in terms of the total internal reflection phenomenon, a detailed analysis of their electromagnetic waveforms involves solving Maxwell’s equations with appropriate boundary conditions [1,2]. For the case of Transverse-Electric (TE) propagation, this would mean the solution of the Helmholtz equation:

$$\nabla^2 \langle E \rangle + (n^2 k^2 - \beta^2) \langle E \rangle = 0 \quad (1)$$

where $\langle E \rangle$ represents the electric field, $n$ is the refraction index, $k$ is the wave number, and $\beta$ is the propagation constant. Appropriate boundary conditions have to be applied for the interfaces of dielectric media with different refraction indices. This is a fairly straight-forward process for a single waveguide with a step-profile of refraction indices $n_s$, $n_f$, and $n_c$ for the substrate, film and cover, respectively [1]. However, changing the distribution of the refraction index can complicate the process severely, often making it impossible to derive an analytical solution. This could, for example, involve a graded index profile, or a periodic structure of adjacent waveguides where the films (through which the waves actually propagate) have an index of $n_f$, with intermediate layers of refraction index $n_i$, where $n_i < n_f$.

Here we consider several cases of such coupled-waveguide structures. The goal is to find out the waveforms (of the electric field) and propagation constants of structures composed of dielectric waveguides placed close enough to each other for their solutions to be different from that of a single waveguide. We will use the tight-binding method from solid state physics for this purpose. It is based on the assumption that the electronic wave functions in structures of several atoms (or generally, potential wells) placed close to each other can be expanded as a linear combination of
the wave functions of the individual atoms. The wave functions of the individual atoms are assumed to be known from the solution of Schrödinger’s equation for a single potential well, and thus the solution for the coupled case is derived by substituting the linear combination into Schrödinger’s equation to find the unknown coefficients [3,4]. In the next section, it will be explained how exactly the same process can be applied to electromagnetic problems consisting of closely placed waveguides which may be called alternating “index profile wells”. The main result of this analysis is the fact that coupled waveguide structures constitute a form of a photonic bandgap material, and that tight-binding can be employed to derive the band structure and waveforms of such a coupled system.

2 Similarity of Schrödinger and Helmholtz Equations

Schrödinger’s (time independent) equation may be written in the following form:

\[ H \psi = E \psi \]  

(2)

in which \( H \) is the Hamiltonian operator, \( E \) represents the energy of the particles concerned, and \( \psi \) is their wave function. Comparing equations (1) and (2), we can re-write (1) with the following definition for the operator \( H \):

\[ H = \nabla^2 + n^2 k^2 \]  

(3)

This similarity of the Helmholtz and Schrödinger equations is because of the boson nature of the photons [5]. The basic equations describing the behavior of electrons in a solid and the behavior of photons in an arrayed waveguide structure (or any photonic bandgap material) are the same. The critical sizes for these phenomena are very different, however. For electrons it is a few angstroms, while for photons it is on the order of a micron. The other difference is that electrons, unlike photons, are fermions, and thus behave differently when occupying the allowed energy states (i.e. the pauli exclusion principle holds for them) [5].

In the next section the tight-binding method is applied to equation (4), which forms the basis for our analysis method.

3 Proposed Analysis Method

For further simplification, one may replace \( \beta^2 \) in equation (4) with a new parameter \( A \) to obtain:

\[ H \langle E \rangle = A \langle E \rangle \]  

(5)

Assuming \( n \) coupled waveguides with individual electric field wave forms \( \langle E_1 \rangle \) to \( \langle E_n \rangle \) and propagation constants \( \beta_1 \) to \( \beta_n \), the tight-binding assumption states:

\[ \langle E \rangle = \sum_{j=1}^{n} a_j \langle E_j \rangle \]  

(6)

The problem is finding the coefficients \( a_i \) for \( \langle E \rangle \) to satisfy (5). Substituting equation (6) into (5) and carrying out an extra multiplication and integration yields:

\[ \sum_{j=1}^{n} a_j \langle E_i \rangle \langle H \rangle \langle E_j \rangle = A \sum_{j=1}^{n} a_j \langle E_i \rangle \langle E_j \rangle \]  

(7)

where \( i \) and \( j \) range from 1 to \( n \) and we have made use of the Dirac notations:

\[ \langle E_i \rangle \langle H \rangle \langle E_j \rangle = \int \langle E_i \rangle \times H \langle E_j \rangle \, dr \]  

(8)

and

\[ \langle E_i \rangle \langle E_j \rangle = \int \langle E_i \rangle \times \langle E_j \rangle \, dr \]  

(9)

Finally, equation (7) can be written in matrix form:

\[
\begin{bmatrix}
\langle E_1 \rangle \langle H \rangle \langle E_1 \rangle & \ldots & \langle E_1 \rangle \langle H \rangle \langle E_n \rangle \\
\vdots & \ddots & \vdots \\
\langle E_n \rangle \langle H \rangle \langle E_1 \rangle & \ldots & \langle E_n \rangle \langle H \rangle \langle E_n \rangle 
\end{bmatrix}
\begin{bmatrix}
a_1 \\
\vdots \\
a_n 
\end{bmatrix}
= A
\begin{bmatrix}
\langle E_1 \rangle \langle E_1 \rangle & \ldots & \langle E_1 \rangle \langle E_n \rangle \\
\vdots & \ddots & \vdots \\
\langle E_n \rangle \langle E_1 \rangle & \ldots & \langle E_n \rangle \langle E_n \rangle 
\end{bmatrix}
\begin{bmatrix}
a_1 \\
\vdots \\
a_n 
\end{bmatrix}
\]  

(10)

This represents an eigenvalue problem with the solutions \( A_1 \) to \( A_n \), which in turn yield \( \beta_1 \) to \( \beta_n \), i.e.
the desired propagation constants. The eigenvectors obtained from this solution give the coefficients $a_i$, and thus the electric field wave form $E$. Terms of the form $\langle E_i | H | E_j \rangle$ are called hoppings, whereas values like $\langle E_i | E_j \rangle$ are called overlaps. Their values are affected by the distance between adjacent waveguides; that is, for completely separated waveguides both hopping and overlap are zero, which makes (10) to reduce to a simple Helmholtz equation for each waveguide. This means the waveguides are completely unaffected by each other. For closely spaced structures, however, (8) and (9) yield values that are not negligible, and one must incorporate first the hoppings, and with decreasing spacing also the overlaps of the wave forms into the calculation. Interestingly, many of the values in each $n \times n$ matrix in (10) will still be zero, because hoppings and overlaps of pairs which are distant enough remain negligible, even with decreasing distance among adjacent waveguides. In a linear array of waveguides, for example, it is concluded that:

$$\langle E_i | H | E_j \rangle_{|j-m|} = 0$$

and:

$$\langle E_i | E_j \rangle_{|j-l|} = 0$$

where $m$ and $l$ are small numbers, typically less than 5.

Eventually, an eigenvalue problem is obtained which is characterized by the $n \times n$ hopping and overlap matrices. This problem may generally be solved numerically. In many cases, however, because of the standard forms these two matrices may take due to the geometry of the problem, closed-form relationships may be derived for the propagation constants of the coupled structures. A number of such examples will be treated in the next sections.

### 4 Linear Array of Waveguides

The first case is a linear array of $n$ adjacent dielectric slab waveguides. As mentioned before, hopping and overlap terms become zero for waveguides that are spaced distant enough from each other. Therefore, depending on the values of $m$ and $l$ in (11) and (12), the hopping and overlap matrices take the forms of multi-diagonal matrices. For the $m=l=1$ case, for example, they become tridiagonal. Assuming similar propagation modes $\beta_0$ for all waveguides, the resulting eigenvalue problem looks like this:

$$\begin{bmatrix}
A_0 & h & 0 & 0 & \cdots & 0 & 0 \\
h & A_0 & h & 0 & \cdots & 0 & 0 \\
0 & h & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & \ddots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & \cdots & 0 & h & A_0 & h \\
0 & 0 & \cdots & 0 & 0 & h & A_0 \\
\end{bmatrix}
\begin{bmatrix}
a_1 \\
\vdots \\
a_n \\
\end{bmatrix} = A
\begin{bmatrix}
1 & \cdots & 0 & 0 & 0 \\
\nu & 1 & \nu & 0 & \cdots & 0 \\
0 & \nu & \ddots & \ddots & \ddots & \ddots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & 0 & \nu & 1 & \nu & \cdots \\
0 & \cdots & 0 & \nu & 1 \\
\end{bmatrix}
\begin{bmatrix}
a_1 \\
\vdots \\
a_n \\
\end{bmatrix}
$$

in which:

$$A_0 = \beta_0^2 = \langle E_i | H | E_j \rangle $$

$$h = \langle E_i | H | E_j \rangle_{|j-l|} $$

$$\nu = \langle E_i | E_j \rangle_{|j-l|} $$

and we have normalized the waveforms so that:

$$\langle E_i | E_j \rangle = 1$$

where $i$ and $j$ range from 1 to $n$.

The solution of this problem involves $n$ eigenvalues $A_i$ to $A_n$ (or $\beta_1$ to $\beta_n$), with each having a corresponding eigenvector with a set of values $a_1$ to $a_n$ from which the electric field waveform can be obtained using (6). The eigenvalues (propagation constants) obtained from (13) can be shown to be [6]:

$$A_m = \beta_m^2 = \frac{\beta_0^2 + 2h \cos(\frac{m\pi}{n+1})}{1 + 2\nu \cos(\frac{m\pi}{n+1})}$$

,  \quad m = 1,2,...,n

(18)
It is interesting to note that for an odd number of waveguides, there is always a propagation constant of the coupled system which is exactly equal to that of each single waveguide. Clearly, this happens for \( m = \frac{n+1}{2} \). An important special case is that of two similar adjacent waveguides. Putting \( n = 2 \) in (18), one obtains:

\[
A_1 = \beta_0^2 = \frac{\beta_0^2 + h}{1 + \nu}, \\
A_2 = \beta_0^2 - \frac{h}{1 - \nu} \tag{19}
\]

If the two waveguides are spaced distant enough, the overlap terms may be neglected and we get \( A_1 = \beta_0 + h \) and \( A_2 = \beta_0 - h \), which reminds us of the familiar results for two adjacent atoms (bonding and anti-bonding orbitals) in quantum mechanics, where energy has been replaced by the squared propagation constant \( A \). The equivalent of an ionic bond would imply the analysis of two waveguides with dissimilar propagation modes. Calling the propagation constants \( \beta_0 \) and \( \beta_{02} \), equation (13) reduces to:

\[
\begin{bmatrix}
A_{01} & h \\
h & A_{02}
\end{bmatrix}
\begin{bmatrix}
a_1 \\
a_2
\end{bmatrix}
= 
\begin{bmatrix}
1 & \nu \\
\nu & 1
\end{bmatrix}
\begin{bmatrix}
a_1 \\
a_2
\end{bmatrix}
\tag{20}
\]

Solving for \( A_1 \), one obtains:

\[
A_1 = \beta_0^2 = \frac{\beta_{01}^2 + h - \nu (\beta_{02}^2 + h)}{1 - \nu^2}, \\
A_2 = \beta_0^2 = \frac{\beta_{02}^2 - h + \nu (\beta_{01}^2 - h)}{1 - \nu^2} \tag{21}
\]

which reduces to (19) if \( \beta_0 \) and \( \beta_{02} \) are the same.

In the next section, another special case will be investigated which is a circular array of adjacent dielectric waveguides.

5 Circular Array of Waveguides

In this section a circular array of waveguides is considered. Obviously, the waveguides have to be channel waveguides rather than slab structures to be placed on a circle. Nevertheless, if the radius of the circle is big enough, only the coupling along the circle’s periphery will be significant and we may still use a one-dimensional analysis such as that for a linear array. The only difference between this case and the linear array is the coupling between the first and \( n \)-th waveguides. Therefore, we will have rotating hopping and overlap matrices rather than tridiagonal ones. Assuming negligible overlaps, equation (13) will change to:

\[
\begin{bmatrix}
A_0 & h & 0 & \cdots & 0 & h \\
h & A_0 & h & \cdots & 0 & 0 \\
0 & h & \cdots & \cdots & \cdots & 0 \\
0 & 0 & \cdots & 0 & 0 & 0 \\
0 & \cdots & \cdots & \cdots & \cdots & 0 \\
h & 0 & \cdots & 0 & 0 & A_0 \\
0 & 0 & \cdots & 0 & 0 & h
\end{bmatrix}
= 
\begin{bmatrix}
a_1 \\
\vdots \\
a_s
\end{bmatrix}
\tag{22}
\]

which can be solved to give [6]:

\[
A_m = \beta_m^2 = \beta_0^2 + 2h \cos\left(\frac{2m\pi}{n}\right), \quad m = 1, 2, \ldots, n \tag{23}
\]

It is interesting to note that in both the linear and the circular arrays (equations (18) and (23)), the maximum range obtained for \( \beta_2 \) is \( 4h \). This value is analogous to the width of the allowed energy bands in a solid, which may also be computed by tight-binding. The bigger the hopping, the bigger is the bandwidth; this is also clear intuitively.

The next section examines the accuracy of the presented method by comparing its results to those of the previously established beam propagation method [7,8].

6 Comparison with BPM

To test the validity of the presented method we consider the case of two adjacent waveguides with similar propagation modes, and compare the results of equation (19) to those of the previously established beam propagation method (BPM) [7,8]. The structure is shown in figure 1. Two dielectric slab waveguides are considered with step-profile refraction indices of \( n_f = 3.380 \) and \( n_i = 3.377 \). The propagating wave has a wavelength of 1.15 µm. For a single waveguide, it can be easily shown that for the first TE mode we have \( \beta_0 = 18.4612 \) µm\(^{-1}\). (We consider only the first TE modes for the purpose of this example.) For the coupled structure of figure 1, BPM yields \( \beta_0 = 18.4603 \) µm\(^{-1}\) and \( \beta_2 = 18.4622 \) µm\(^{-1}\); whereas using (19), one obtains \( \beta_0 = 18.4601 \) µm\(^{-1}\) and \( \beta_2 = 18.4621 \) µm\(^{-1}\) which is fairly similar to the BPM results. To evaluate (19), we have computed the hopping and overlap values.
from numerical integration of (8) and (9) using the (known) waveforms for the electric field. These values have been 60.7706 µm⁻² for hopping and 0.1782 µm⁻² for overlap. A clear advantage of the tight-binding approach is that it gives not only the propagation constants, but also the waveforms of the coupled structure, although the waveforms have not been considered here.

7 Other Examples of employing Tight-Binding in Photonics

The idea of using the tight-binding approach to analyze problems in optics and electromagnetics is not new. This work, however, is to the best of our knowledge the first demonstration of the usefulness of tight-binding in describing coupled dielectric waveguide structures.

In [9,10], tight-binding has been successfully employed to study coupled microcavities introduced into a photonic crystal by intentionally adding defects to it. For a high enough density of defects, a defect band is introduced into the band structure obtained for the propagation constants of the system. In the next section a similar effect will be shown to exist in a coupled waveguide structure. In [11] it is explained how such a system can be used to design filters, which is also an obvious application of the coupled waveguide structures presented here. Knowledge of the allowed and forbidden propagation modes can be obtained by tight-binding and applied to the design of the filters.

Coupled resonator optical waveguides have been successfully analyzed in [12]. In [13], the tight-binding method is shown to be useful in analyzing a two-dimensional photonic crystal by comparing it to ab initio results. In [14], the concept of adding defect levels into the band structure of a photonic crystal in a manner analogous to doping in semiconductors is clarified. The next section presents the similar phenomenon in a coupled waveguide system by a number of examples.

8 Simulation Examples – Effect of Defects on the Band Diagram

Example 1 – We consider a linear array of 18 similar adjacent dielectric waveguides. The fundamental propagation constants for a single waveguide are assumed to be 2µm⁻¹ and 3µm⁻¹. The hoppings are assumed to be first-level only (i.e. just among adjacent waveguides) and to be equal to 0.2µm⁻² and 0.5µm⁻² for the first and second modes, respectively. Overlaps are neglected. These values are empirical and only serve the purpose of illustration.

Filling out the appropriate terms in the hopping matrix of equation (13) and letting MATLAB solve the eigenvalue problem, the allowed propagation constants of the system take the form of figure 2. The band structure and splitting of allowed propagation constants is clearly evident from the figure. The result is that the coupled waveguide structure forms a photonic bandgap. Note that the vertical axis gives the allowed propagation constants, and the horizontal axis does not represent any physical quantity. It has only been added to better illustrate the allowed and forbidden bands for the propagation constant.

Example 2 – Imperfections in the array may cause single rows of the hopping matrix in equation (13) to be different from the rest. The result of a MATLAB simulation is shown in figure 3. A defect state with a slight split can be observed due to one dissimilar waveguide in the array having a fundamental propagation constant of 2.5. The split can be attributed to the weak interaction
of the defect mode with the main modes of the other waveguides.

Example 3 – Finally, the simulation result shown in figure 4 demonstrates a defect band instead of a defect state, due to the increased number of (five) defected waveguides. These results are reminiscent of the numerical and experimental results presented in [9,10], though they refer to a different phenomenon, namely, coupled microcavities instead of coupled waveguides.

Figure 3: Allowed propagation constants (μm⁻¹) for a linear array of 18 waveguides with one defect.

Figure 4: Allowed propagation constants (μm⁻¹) for a linear array of 18 waveguides with five defects.

9 Conclusions

The tight-binding approach was employed to analyze coupled dielectric waveguide structures. This has been motivated by the similarity of the Schrödinger and Helmholtz equations. Closed-form solutions were derived for linear and circular arrays of adjacent slab waveguides and computer simulation was used to compare the results to the beam propagation method. Examples were presented to demonstrate the effect of defects on the obtained propagation band diagram.

References