# ALGORITHMS FOR THE SOLUTION TO THE HELMHOLTZ EQUATION IN THE NUMERICAL SIMULATION OF SEMICONDUCTOR LASERS.

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## Abstract

In the numerical simulation of semiconductor lasers a fast accurate method is essential for the solution to the Helmholtz equation. Various algorithms are considered for this purpose in terms of speed, efficiency and accuracy and a new algorithm is developed based on the effective index method with a novel solution to the algebraic eigenvalue equation. The algorithm is found to be highly efficient for all modes.

## **I. Introduction**

As laser structures increase in complexity it becomes more important to simulate their behaviour in order to understand phenomena dependent on structure and hence optimise their performance. As manufacturing techniques improve the buried heterostructure (BH) device is likely to grow in importance. A typical BH device is shown schematically in figure 1 in which the InGaAsP active region is surrounded by the wider band gap InP on all sides. In the simulation of these structures the wave equation must be solved to obtain the optical intensity of each lasing mode and the aim of this paper is to investigate the most efficient way to solve this equation.



Figure 1 Device Structure

## **II.** Modelling

Assuming TE modes dominate then the wave equation may be given in scalar form as

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \varepsilon(x, y)k_o^2 - \beta^2\right)E_x = 0$$
(1)

where  $\varepsilon(x,y)$  is the permittivity (which may be complex due to gain or loss),  $E_x$  is the optical field,  $k_o$  is the free space wave number and  $\beta$  is the propagation constant. This equation must be solved in two

dimensions for the structure in figure 1. Of the efficient methods that exist the effective index method [1] is the most commonly used, however as the active area decreases in size and the solution approaches cut-off the accuracy deteriorates [2]. The weighted index method [3] is an alternative approach which attempts to increase the accuracy of the solution whilst avoiding the complexity of a two-dimensional method.

### The Weighted Index Method

The weighted index method is an improvement on the effective index method as it uses a weighted mean of the permittivities in the y direction for each node in the x axis and a weighted mean of the permittivities in the x direction for each node in the y axis. This is described with reference to figure 2.



### Figure 2 The Weighted Index Method

The best trial solution is found for

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$$\mathbf{E} = \mathbf{F}(\mathbf{x})\mathbf{G}(\mathbf{y}) \tag{2}$$

F and G are complex functions of the single variables x and y respectively and satisfy the ordinary differential equations

$$\frac{d^2F}{dx^2} + K_F F = \beta_x^2 F$$
(3)

$$\frac{d^2G}{dy^2} + K_G G = \beta_y^2 G$$
(4)

where  $\beta_x$  and  $\beta_y$  are the propagation constants of the differential equations. Equation 3 represents a cut along aa' and equation 4 represents a cut along bb'. There are p nodes along the aa' and q nodes along bb'. K<sub>F</sub> is the weighted mean of  $\varepsilon(x, y)k_o^2$  for each nodal value  $x_p$ . The mean is taken along the y direction using weights  $w_{yq}$ , i.e.

$$K_{F} = k_{o}^{2} \sum_{q} w_{yq} \varepsilon_{pq}$$
<sup>(5)</sup>

In a similar fashion  $K_G$  is given by

$$K_{G} = k_{o}^{2} \sum_{p} w_{xp} \varepsilon_{pq}$$
(6)

The weights are defined optimally as

$$w_{xp} = \int_{x_p}^{x_{p+1}} F^2 dx$$
(7)

$$w_{yq} = \int_{y_q}^{y_{q+1}} G^2 dy$$
 (8)

where F and G have undergone the normalisation

$$\int_{-\infty}^{\infty} \mathbf{F}^2 = 1 \tag{9}$$

$$\int_{-\infty}^{\infty} G^2 = 1 \tag{10}$$

The best value of  $\beta^2$  is given by the Rayleigh quotient [3]

$$\beta^{2} = \beta_{x}^{2} + \beta_{y}^{2} - k_{0}^{2} \sum_{p} \sum_{q} w_{xp} w_{yq} \varepsilon_{pq}^{2}$$
(11)

The two one-dimensional wave equations (3,4) are coupled via the weighting factors and are solved alternately until the value for  $\beta$  converges.

#### The algebraic eigenvalue equation

With both the effective and weighted index methods a one dimensional algebraic eigenvalue equation must be solved.

$$\mathbf{A}\mathbf{E} = \boldsymbol{\beta}^2 \mathbf{E} \tag{12}$$

where A is complex and tridiagonal and the optical field E is a column vector. If a non-uniform grid is used then A is unsymmetrical and must be symmetrised using a similarity transformation. The eigenvalue and eigenfunction of the coefficient matrix A give the propagation constant  $\beta$  and the corresponding optical field E respectively. A new highly efficient method is described next.

### **Evaluation of the characteristic polynomial**

A very fast method to obtain any required eigenvalue is the evaluation of the characteristic polynomial. A trial value of the eigenvalue is used in a Sturm sequence which can then be used to locate the required eigenvalue via bisection. For any trial eigenvalue  $\lambda$ , the Sturm sequence is defined as :-

$$p_{o}(\lambda) = 1$$
  

$$p_{i}(\lambda) = (a_{ii} - \lambda)p_{i-1}(\lambda) - a_{ij}^{2}p_{i-2}(\lambda)$$
(13)

The number of changes in sign between consecutive numbers of the sequence is equal to the number of eigenvalues smaller than  $\lambda$ . The advantage of this method is its flexibility in that it allows all the eigenvalues to be found in a given range however the disadvantage is it cannot cope with complex matrices.

An alternative method is inverse power iteration with successive eigenvalue refinement. It consists of iterating around the equation

$$(\mathbf{A} - \boldsymbol{\mu}_i \mathbf{I}) \mathbf{x}_{i+1} = \mathbf{k}_i \mathbf{x}_i \tag{14}$$

where  $k_i$  is chosen such that  $\|\mathbf{x}_{i+1}\|_{\infty} = 1$ .  $\mu_i$  is adjusted on each iteration via

$$\mu_{i+1} = \mu_i + \frac{1}{k_i}$$
(15)

A linear system of equations must be solved at each step. This algorithm is fast and can cope with complex eigenvalues and eigenvectors. The main disadvantage is that the method requires good approximations to both the eigenvalue and the eigenvector of the problem to initialise. However advantage can be taken of the fact that the change in imaginary components of the permittivity is much less than the change in real components. This is due to the BH laser being index-guided in both lateral and transverse directions. To obtain a good initial approximation to the complex problem the imaginary components can be ignored and the real problem can be solved via the evaluation of the characteristic polynomial for the eigenvalue and an inversion performed for the eigenvector. The results can then be used to initialise the complex inverse iteration with successive eigenvalue refinement algorithm to obtain the complex solution. A flowchart of the algorithm is shown in figure 3



Figure 3 Flow Chart of Operation

## **III.** Results and Discussion

Results are shown in figure 4 for an InGaAsP/InP device using the effective index Method (EI), the Weighted Index Method (WI) and a two-dimensional solution (2D)[2]. The fundamental and first order mode indices are calculated for varying channel widths (W). In this example where the core is 0.35 microns thick the effective index method becomes significantly in error when the width is less than two microns i.e. when the active region area is less than approximately 0.6  $\mu$ m<sup>2</sup>.

The significance of the above results will now be considered with respect to the design of BH lasers. One of the most important characteristics of these devices is the power at which the first kink in the light-current characteristics occurs. This kink is due to the first order mode achieving gain and commencing lasing. The above results indicate that for accurate determination of this lasing power the EI method is insufficient and the WI method is preferred. An interesting implication of the results given in figure 4 is that the EI method will always underestimate the optical power at which the first order mode starts to lase and the weighted index method will always overestimate this power. This is a direct result of the effective index method overestimating the mode index and hence overestimating the optical gain. Equivalently, the weighted index underestimates the mode index and thereby underestimates the optical gain. This has important implications for device engineers. If a laser is designed to have a minimum output power at which the first order mode starts to lase, then using both the WI and EI methods, they can be reasonably sure that the experimental power will be bounded by the results calculated from the two methods.



Figure 4 Typical Result



### References

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