

Solution Procedure for a Class of Band Structures – Application of the Finite Element Method to Schrödinger's Equation

Najib A. Kasti

Department of Mechanical Engineering, Taibah University, Saudi Arabia

najib01@idm.net.lb

Abstract- Several publications used the finite element method to determine the band structures of periodic solids by solving the Schrödinger equation (for example, Pask et al., Sukumar et al. [1-4]).

The approaches used by these publications could basically be divided into two. The first approach (Pask et al. [1-3]) expresses the wave function ψ as the product of a harmonic function and a periodic function using Bloch's theorem. The periodic function is then discretized over the domain.

In contrast, the second approach (Sukumar et al. [4]) discretizes the wave function over the domain with its nodal values being complex in this case.

This paper discusses a solution procedure for determining the band structures for a class of materials starting from the approach followed by Sukumar [4]. It assumes that one can obtain the discrete Hamiltonian and overlap matrices from a conventional finite element analysis program without reverting to a special program. The application of the boundary conditions and the solution of the band structures, for the defined class of material, are performed through matrix operations of well defined steps. The final complex eigenvalue problem, to determine the band energies of the system, is then solved by conventional methods.

When solving the resulting system, two representations of the overlap matrix were tested in this work, namely, the consistent and lumped representations. Each of these representations displayed a different response when compared to the exact solution. The results from the lumped and consistent formulations as well as those from a simple averaging process are discussed in this paper.

Keywords- Quantum Mechanics; Finite Element Method; Schrödinger Equation; Periodic Solids

I. INTRODUCTION

Determining the band structures of periodic solids involve solving the Schrödinger's equation with an equivalent potential and periodic boundary conditions [1-4].

Different methods could be used for such a task, such as the Fourier analysis and the finite element method, among others. Within the class of finite element solution methods, the work of Pask et al. [1-4] and Sukumar et al. [4] are mostly quoted in this paper.

Pask et al. [1-3] start with the Schrödinger equation, and using Bloch's theorem, replace the wave function by the product of a harmonic function and a periodic function. Inserting the above decomposition into the differential equation and using the weak form results in a complex finite element formulation. In this case, the interpolation functions of the periodic function are real.

On the other hand, Sukumar et al. [4] use the wave function as the main variable in the finite element formulation and thus the variables at the nodes are complex wave function values.

In this paper, we start with the basic equation of quantum mechanic and use the wave function as the main variable, similar to the work presented by Sukumar [4]. However, instead of developing a special finite element program to solve the resulting formulation, we proceeded as follows. First, we assumed that the discrete Hamiltonian and overlap matrices are obtained from a conventional finite element program (like the conductivity and mass matrices), and thus there is no need to develop a special program to compute them. Second, the periodic boundary conditions were applied through matrix operations of well-defined steps. Thirdly, we selected the class of materials for which the special periodic boundary mesh renders the "force" vector null. Fourthly, this led us to a regular complex-eigenvalue problem that is solved to determine the system energies. In the finite element formulation, two presentations for the overlap matrix were used, namely, the consistent and lumped representations. The effects of each as well as those from a simple averaging process were discussed. The paper concludes with examples to validate the procedure proposed.

The advantages of the above procedure may be summarized as follows. a-The discrete Hamiltonian and overlap matrices can be computed by using the meshing/computation capabilities of conventional finite element programs. Also, the mesh refining capabilities of these programs can be utilized. This is made possible since the periodic boundary conditions are applied from outside the formulation through matrix operations and not built into the formulation a priori. b-The compact finite

element formulation presented and the matrix application of the periodic boundary conditions may facilitate the development of an error analysis scheme. c-Without a mesh refinement, an averaging process is presented, which may lead to an improvement in the error analysis.

II. BLOCH THEOREM FOR PERIODIC SOLIDS AND THE PERIODIC BOUNDARY CONDITIONS

Felix Bloch discovered that the wave function $\Psi(r)$ in the Schrödinger equation for periodic solids with periodic potentials is equal to a periodic function $u(r)$ multiplied by a harmonic function $e^{ik \cdot r}$, where r and k are the electron position and Bloch's wave vector, respectively. One can prove that the above statement is equivalent to having the wave function $\Psi(r)$ satisfying $\Psi(r+R) = e^{ik \cdot R} \Psi(r)$, where R is the periodicity or lattice translation vector of the solid [5]. When the periodic boundary conditions are applied to the solution to the Schrödinger equation for periodic solids, the wave vector k is quantized.

III. REVIEW OF SOME METHODS USED TO SOLVE THE SCHRÖDINGER EQUATION FOR PERIODIC SOLIDS

The stationary expression of the Schrödinger equation for a many-body problem [6] can be expressed as:

$$\hat{H} \Psi = [T_n + T + U_n + U + V] \Psi = E_T \Psi, \quad (1)$$

where T_n = kinetic energy of the nuclei

T = kinetic energy of the individual electrons

U_n = nucleus-nucleus interaction term

U = electron-electron interaction term

V = interaction of electrons and nuclei term

E_T = total energy

Ψ = wave function

Using the Born-Oppenheimer approximation, the solution of the nuclei motion can be decoupled from the electrons motion, and the equation simplifies to:

$$H\Psi = [T + U + V]\Psi = E\Psi, \quad (2)$$

where E is the electronic energy.

The density functional theory (DFT) attempts to solve the many-body problem by replacing it with a one-electron problem (or many non-interacting electrons) subjected to a potential that represents the combined effects of U and V above [7]. For periodic solids [8], the valence electron may be assumed to be non-interacting and subjected to a periodic potential (which is a result of the interaction with the ions and a mean field from the other electrons). This decouples the Schrödinger equation into a system of single-electron equations. The adequacy of the solution depends on the qualitative representation of the periodic potential. Accurate potentials, justified by DFT for example, would lead to better solutions [9].

The above assumption, of non-interacting valence electrons subjected to a resultant periodic potential, was taken in this work. Thus, for the case of one-electron problem, the Schrödinger equation can be written as:

$$-\left(\frac{h^2}{2m}\right)\nabla^2\Psi + V\Psi = E\Psi, \quad (3)$$

where $h=1.0545 \times 10^{-34}$ J.s. is the Planck's constant divided by 2π , m is the mass of the particle (in this case the electron), Ψ the wave function, V the equivalent periodic potential and E the electron energy.

Five methods/procedures for solving this equation were referred to in this paper, namely:

- 1) Closed form solution, when possible;
- 2) Fourier series solution;
- 3) Method of Pask [1-3] where the wave function is replaced in the Schrödinger equation by a complex harmonic part $e^{ik \cdot r}$ and a periodic function $u(r)$;
- 4) Method of Sukumar [4] where the wave function is used as the basic variable, and the boundary conditions are applied at the periodic nodes; and
- 5) The procedure described below.

In the following section, a complimentary procedure for solving the Schrödinger equation for a class of periodic solids is presented.

IV. PROPOSED PROCEDURE FOR SOLUTION

A. Schrödinger Equation – Normalized (Dimensionless) Form

The one-electron Schrödinger equation can be written as

$$-\left(\frac{h^2}{2m}\right)\nabla^2\Psi + V\Psi = E\Psi \quad (4)$$

If the coordinates X, Y and Z are also normalized with a_0 (a basic unit of length), and if we let $E^* = 2m \cdot a_0^2 E/h^2$ and $V^* = 2m \cdot a_0^2 V/h^2$, then, the resulting normalized Schrödinger equation can be expressed as:

$$-\nabla^2\Psi + V^*\Psi = E^*\Psi \quad (5)$$

B. Weak Form of the Schrödinger Equation

Applying the weak form [10] to Schrödinger's equation results in

$$\int_{\Omega} \mathbf{v}^* [-\nabla^2\Psi + V^*\Psi - E^*\Psi] d\Omega = 0 \quad (6)$$

where $\mathbf{v}^*$ is the complex-conjugate of the trial function $\mathbf{v}$ which has the same interpolation functions as Ψ in these derivations.

Integration of Eq. (6) by parts leads to

$$\int_{\Omega} [\nabla \mathbf{v}^* \cdot \nabla \Psi] d\Omega + \int_{\Omega} [V^* - E^*] \mathbf{v}^* \Psi d\Omega = \int_{\Gamma} \mathbf{v}^* (\nabla \Psi \cdot \mathbf{n}) d\Gamma \quad (7)$$

C. Periodic Boundary Conditions

The periodic boundary conditions are specified as [1-4]

$$\Psi(\mathbf{r} + \mathbf{R}) = e^{ik \cdot \mathbf{R}} \Psi(\mathbf{r}), \quad (8)$$

and

$$\nabla \Psi(\mathbf{r} + \mathbf{R}) \cdot \mathbf{n}(\mathbf{r}) = e^{ik \cdot \mathbf{R}} \nabla \Psi(\mathbf{r}) \cdot \mathbf{n}(\mathbf{r}) \Rightarrow \nabla \Psi(\mathbf{r} + \mathbf{R}) \cdot \mathbf{n}(\mathbf{r} + \mathbf{R}) = -e^{ik \cdot \mathbf{R}} \nabla \Psi(\mathbf{r}) \cdot \mathbf{n}(\mathbf{r}),$$

where $\mathbf{R}$ is the lattice translation vector.

D. Finite Element Formulation

Using the standard finite element formulation to the weak form of the Schrödinger equation leads to the following system of equations.

$$\mathbf{K}\Psi - E^* \mathbf{M}\Psi = \mathbf{F}, \quad (9)$$

where

$$\mathbf{K} = \int_{\Omega} \nabla \mathbf{N} \cdot \nabla \mathbf{N}^T d\Omega + \int_{\Omega} \mathbf{V}^* \mathbf{N} \cdot \mathbf{N}^T d\Omega, \quad (10)$$

$$\mathbf{M} = \int_{\Omega} \mathbf{N} \cdot \mathbf{N}^T d\Omega, \quad (11)$$

$$\mathbf{F} = \int_{\Gamma} \mathbf{N} (\nabla \Psi \cdot \mathbf{n}) d\Gamma, \quad (12)$$

Ψ =vector of nodal wave functions, and

$\mathbf{N}$ =shape function vector.

Matrix $\mathbf{K}$, the discrete Hamiltonian matrix, has a parallel in another branch of science, namely, a combination of the “conductivity” and “mass-heat capacity” matrices with the “density” ρ playing the role of the equivalent potential V^* , which is

given in this case. Matrix M , the overlap matrix, is equivalent to the “mass-heat capacity” matrix with density $\rho = 1$. Thus, K and M can be generated from a conventional finite element program once a mesh is built.

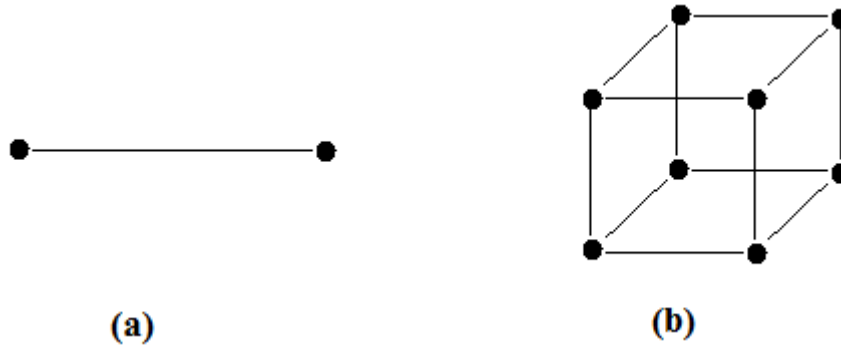


Fig. 1 Elements used in the finite element solution (a) 1D 2-node element. (b) 3D 8-node hexagonal element

In the 1D problem, 2-node C^0 elements were used, as shown in Fig. 1(a) above.

On the other hand, for 3D problems, 8-node C^0 hexagonal elements were used, as shown in Fig. 1(b).

E. Solution Procedure

To solve the above system of equations with periodic boundary conditions, which are complex in this case, and without reverting to a new finite element program, we proceed as follows.

Let n be the total number of nodes and m the number of independent nodes;

Define $\Psi = Ay$ where Ψ ($n \times 1$) is the nodal wave function vector, y ($m \times 1$) is the wave function vector where the dependent nodes are replaced by the independent ones, and A ($n \times n$) a diagonal matrix, part of it relates the dependent degrees of freedom on the boundary to the independent ones through factors of the form $e^{ik.R}$. The other diagonal entries of A would have a value of 1;

For example, assume I as an independent node and J a node that depends on node I . The J -th row of A will be all zeros except the entry $A(I,J)$ which will have a value equals to $e^{ik.R_{IJ}}$;

Let $y = Xz$ where X ($n \times m$) is a matrix, made of 1s and 0s, that relates the modified total nodal wave function vector to the vector of independent degrees of freedom;

Thus, the vector z ($m \times 1$) represents the independent nodal wave function vector.

For example, for the dependent node J , the $X(J,I)$ entry in the matrix X will have a value of 1 and all other entries will be zero.

Actually, matrices A and X could be combined into a single matrix. However, they are preserved here in these forms to explain their individual original roles whereby matrix A was used to apply the periodic boundary conditions and matrix X to add the rows and columns of the equations.

Applying these transformations to Eq. (9) leads to

$$(X^T \cdot A^* \cdot K \cdot A \cdot X) \cdot z - E^* (X^T \cdot A^* \cdot M \cdot A \cdot X) \cdot z = X^T \cdot A^* \cdot F \quad (13)$$

Let $L = X^T \cdot A^* \cdot K \cdot A \cdot X$ and $P = X^T \cdot A^* \cdot M \cdot A \cdot X$, then Eq. (13) can be written as

$$L \cdot z - E^* P \cdot z = X^T \cdot A^* \cdot F, \quad (14)$$

where matrices L and P are complex values.

As is obvious from the above formulation, the resulting matrices are Hermitian, and consequently, the energy eigenvalues are real.

By setting $z = P^{-1/2} \cdot w$ in the above result, Eq. (14) can then be transformed into

$$P^{-1/2} \cdot L \cdot P^{-1/2} \cdot w - E^* \cdot I \cdot w = 0. \quad (15)$$

The resulting equation is a regular complex-eigenvalue problem.

F. Some Properties of the Resulting Matrices

Diagonal matrix A can be decomposed into a real diagonal matrix A_R with values of “1” and “ $\cos(k.R)$ ” terms and another

real diagonal matrix AC with values of “0” and “sin(k.R)” terms. AR represents the real part and AC represents the complex part. Thus, we can write $A = AR + i*AC$.

Then,

$$X^T . A^* . K . A . X = X^T . (AC^T . K . AC + AR^T . K . AR) . X + i * [X^T . (AR^T . K . AC - AC^T . K . AR) . X], \quad (16)$$

and

$$X^T . A^* . M . A . X = X^T . (AC^T . M . AC + AR^T . M . AR) . X + i * [X^T . (AR^T . M . AC - AC^T . M . AR) . X]. \quad (17)$$

It is not difficult to show that the real part of the second term on the right in the above two equations is a skew-symmetric matrix.

The solution to the above eigenvalue problem, using the finite element method, is supposed to provide upper bounds to the energy eigenvalue.

Indeed, the results obtained in this paper were either close to the exact solution or upper bounds.

In this study, we did also attempt to use the concept of “lumped” overlap matrix, as generally applied in structural dynamics to the mass matrix. The terms in each row of the overlap matrix M were summed and placed on the diagonal. This results in an overlap matrix that is an identity matrix for this case of 3D C^0 hexagonal elements. One implication of lumping the overlap matrix is that the right hand side of Eq. (17) is real in this case.

Returning to the formulation at hand, and for the class of problems we are dealing with in this paper, one can prove that the right hand side of Eq. (14) is zero. This is accomplished as follows.

Proposition: For periodic solids with the unit cells meshed using the finite element method, if points on opposing periodic boundary elements have the same lattice translational vector R, then the right-hand side of Eq. (14), namely the vector $Q = X^T . A^* . F$, is a zero vector.

Proof: Assume the independent boundary node **I**, attached to element Γ_I as shown in Fig. 2 below, faces node **J** attached to element Γ_J , on the periodic boundary;

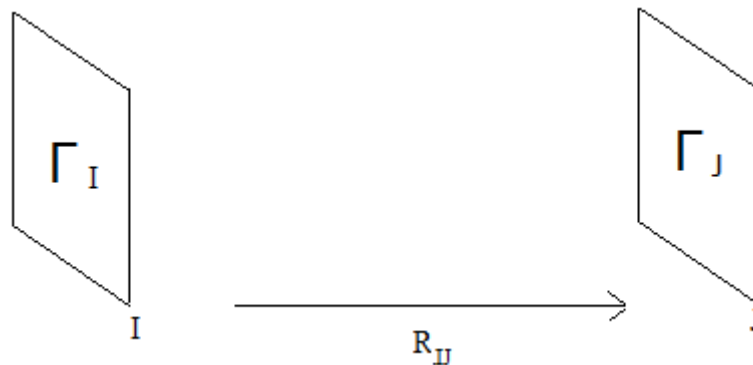


Fig. 2 Boundary elements attached to nodes **I** and **J**

The $Q(I) = X^T A^* F(I)$ entry will involve a sum of integrals over all elements on the boundary that are either attached to node **I** or related to node **I** through the periodicity of the solid.

$$Q(I) = \int_{\Gamma_I} N_I (\nabla \Psi(r) . n(r)) d\Gamma + e^{-ik \cdot R_{IJ}} \int_{\Gamma_J} N_J (\nabla \Psi(r + R) . n(r + R)) d\Gamma + \dots, \quad (18)$$

when Eq. (8b) is substituted in the above equation, we get

$$Q(I) = \int_{\Gamma_I} N_I (\nabla \Psi(r) . n(r)) d\Gamma + e^{-ik \cdot R_{IJ}} \int_{\Gamma_J} N_J (-e^{ik \cdot R} \nabla \Psi(r) . n(r)) d\Gamma + \dots \quad (19)$$

Since by the requirement of the proposition that all points in element Γ_J are related to the opposing points in element Γ_I through the same translational vector R_{IJ} , and since element Γ_I is similar to element Γ_J , then

$$Q(I) = \int_{\Gamma_I} N_I (\nabla \Psi(r) . n(r)) d\Gamma - e^{-ik \cdot R_{IJ}} . e^{ik \cdot R_{IJ}} \int_{\Gamma_I} N_I (\nabla \Psi(r) . n(r)) d\Gamma + \dots = 0 \quad (20)$$

Thus, this proves that for independent boundary nodes, the corresponding entries in the vector **Q** are zero. For interior nodes, the boundary integrals are obviously zero. This implies that the **Q** vector is a zero vector.

Note: Sukumar et al. [4] arrived at a similar conclusion by restricting the test function in the finite element formulation to a special value-periodic subspace.

V. VALIDATION OF RESULTS

To validate the above method of solution, the 1D and 3D Kronig-Penney models were solved.

A. 1D Kronig-Penney model:

In this problem, the electron is subjected to a periodic potential as shown in Fig. 3 below. The values of the parameters used are as follows:

$V_0=100$ Ry, $a=2$ a.u. and $b=0.022$ a.u.

Table 1 compares the results obtained from solving the differential equation for the 1D Kronig-Penney model [11] and the results obtained from the finite element formulation, as presented in this paper. The locations of the solution points E1 through E12 are shown in the plot of energy versus wave number k of Fig. 4. The number of elements used in the finite element mesh was 208 C0 elements. The agreement between the two methods is very good.

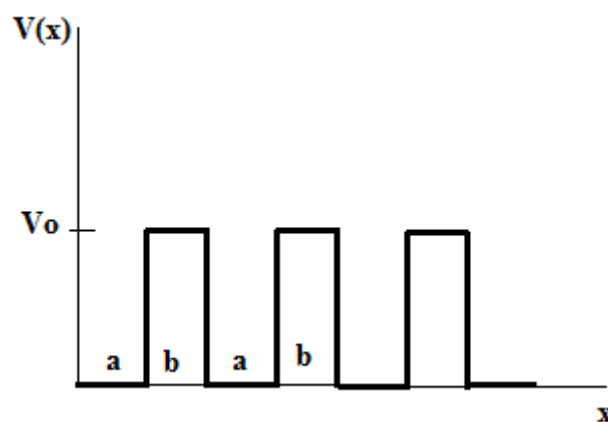


Fig. 3 1D Kronig-Penney periodic potential V versus position x

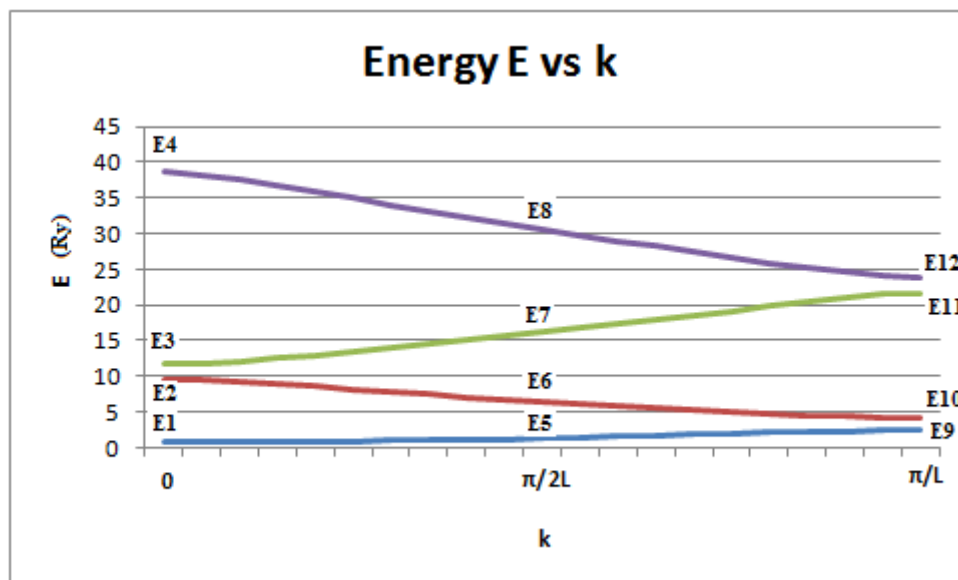


Fig. 4 Energy bands for the 1D Kronig-Penney model. Solution points E1 through E12 correspond to the Finite Element Method

TABLE 1 ENERGIES (RY) FOR THE 1D KRONIG-PENNEY MODEL, EXACT RESULTS VERSUS THE FINITE ELEMENT SOLUTION

K=0	E1	E2	E3	E4
EXACT	0.786	9.657	11.680	38.627

Current FEM work	0.786	9.658	11.681	38.640
-------------------------	-------	-------	--------	--------

K=$\pi/2L$	E5	E6	E7	E8
EXACT	1.334	6.424	16.140	30.644
Current FEM work	1.334	6.424	16.142	30.652

K=π/L	E9	E10	E11	E12
EXACT	2.414	4.182	21.728	23.832
Current FEM work	2.414	4.183	21.732	23.837

B. Generalized 3D Kronig-Penney Model – Simple Cubic Structure

Since the simple cubic structure belongs to the class of problems discussed above, the suggested procedure of solution is applied to this problem.

We used the Generalized 3D Kronig-Penney model, which is a 3D extension of the 1D Kronig-Penney model. The equation of the potential is expressed as:

$$V(x,y,z)=V_{1D}(x)+V_{1D}(y)+V_{1D}(z).$$

The model parameters used were: $V_0=6.5$ Ry, $a=2$. a.u., and $b=1.0$ a.u. [1-3]

Three different methods were used to obtain the band structures, namely

- 1) An 11x11x11 Fourier series solution (taken to be very close to exact and formulated by the author);
- 2) A 12x12x12 C^0 finite element solution using consistent overlap matrix; and
- 3) A 12x12x12 C^0 finite element solution using lumped overlap matrix.

The results are plotted in Fig. 5. As expected, one observes that for a given mesh, the finite element solution with consistent overlap matrix was producing energy values above the “exact” Fourier series solution. On the other hand, the “lumped” overlap solution was giving energy values, in most cases, below the exact values.

Thus, it is tempting to use some kind of averaging on the two solutions obtained with the finite element method. A simple averaging process was attempted and the percentage relative errors of the above three procedures were compared with the Fourier series solution and are plotted in Fig. 6 below. It can be concluded that, in general, the averaging process provides a better solution than the other two methods.

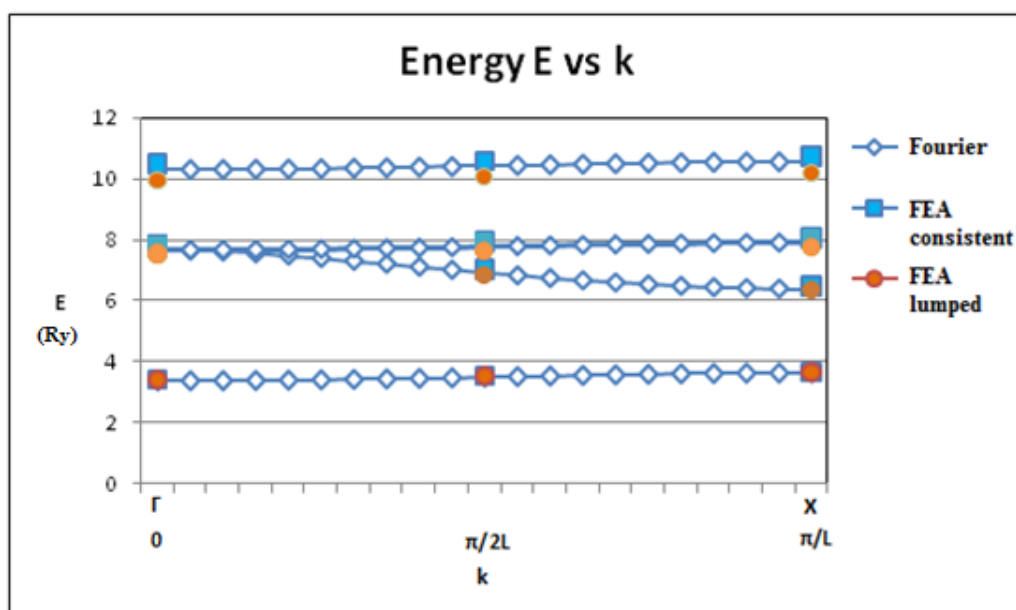


Fig. 5 Band structures for the Generalized 3D Kronig-Penney model (a) Fourier series solution with 11x11x11 terms (b) 12x12x12 C^0 hexagonal elements – Finite element with consistent overlap (c) 12x12x12 C^0 hexagonal elements – Finite element with lumped overlap

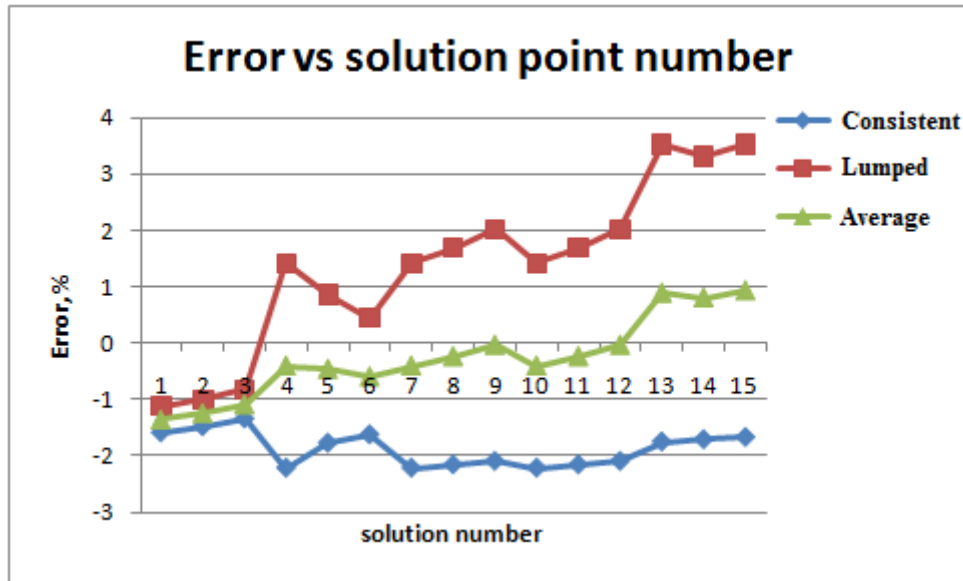


Fig. 6 Errors in the energy for the Generalized 3D Kronig-Penney model relative to the Fourier analysis: (a) Finite element analysis with consistent overlap; (b) Finite element analysis with lumped overlap; (c) Averaging of (a) and (b)

C. Modified 3D Kronig-Penney Model – Simple Cubic Structure

A modified 3D Kronig-Penney model, as it applies to the simple cubic structure, was solved in this paper. This model involves applying a potential around each atom consisting of a cube with constant potential V_0 . The parameters of the problem are as follows: $V_0=6.5$ Ry, $a=2$ a.u., and $b=0.995$ a.u.

Again, the band structures were obtained using an $11 \times 11 \times 11$ Fourier series solution in addition to a mesh of $12 \times 12 \times 12$ C^0 hexagonal elements were the overlap matrix was used as consistent and lumped.

The results, similar to the ones discussed above, are plotted in Figs. 7 and 8.

Also in this case, the consistent overlap matrix was producing energy values above the “exact” Fourier series solution while the “lumped” overlap solution was lower, in most cases. In addition, the averaging solution consistently performed the best.

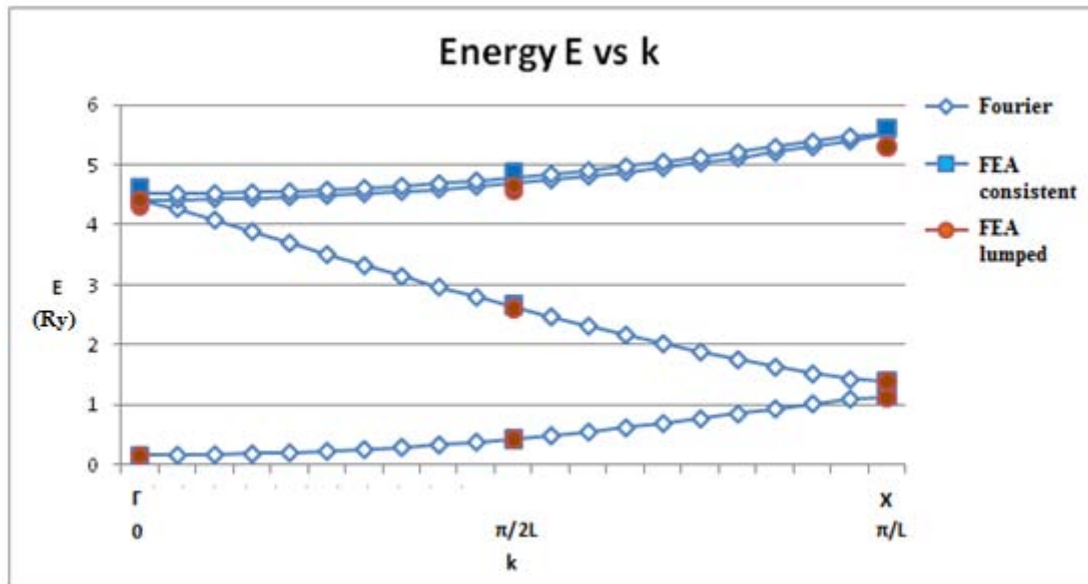


Fig. 7 Band structures for the Modified 3D Kronig-Penney model: (a) Fourier series solution with $11 \times 11 \times 11$ terms (b) $12 \times 12 \times 12$ C^0 hexagonal elements – Finite element with consistent overlap (c) $12 \times 12 \times 12$ C^0 hexagonal elements – Finite element with lumped overlap

To validate the convergence of the finite element solution with mesh refinement, the results from the finite element meshes of $6 \times 6 \times 6$ and $12 \times 12 \times 12$ C^0 hexagonal elements were compared with the Fourier series solution. The results are plotted in Fig. 9. Indeed, refining the mesh does converge the finite element solution to the Fourier analysis.

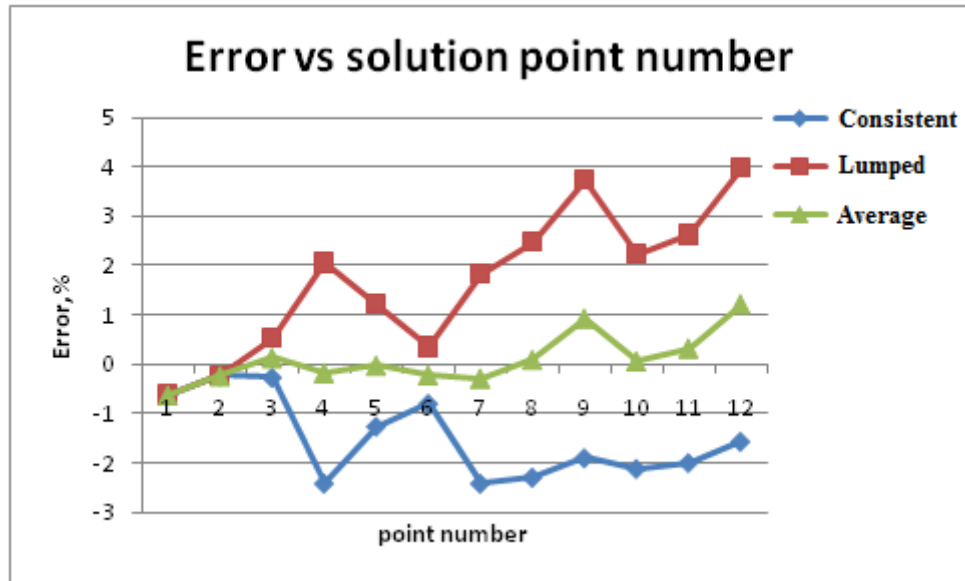


Fig. 8 Errors in the energy for the Modified 3D Kronig-Penney model relative to the Fourier analysis: (a) Finite element analysis with consistent overlap; (b) Finite element analysis with lumped overlap; (c) Averaging of (a) and (b)

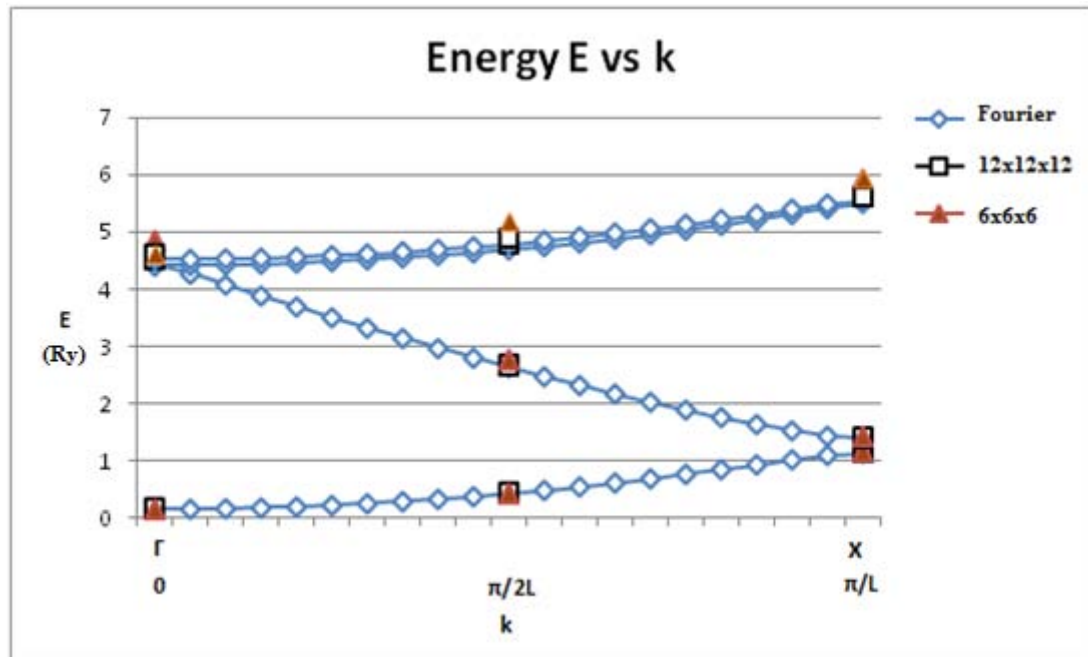


Fig. 9 Band structures of the Modified 3D Kronig-Penney model: (a) Fourier series solution with 11x11x11 terms (b) 12x12x12 C^0 hexagonal elements – Finite element with consistent overlap (c) 6x6x6 C^0 hexagonal elements – Finite element with consistent overlap

VI. CONCLUSIONS

A solution procedure was presented; it determines the band structures for a class of periodic solids where the boundary integral, in the finite element formulation, vanishes. On the other hand, if the boundary integral does not vanish, the solution procedure could be modified by updating the discrete Hamiltonian and overlap matrices, accordingly. Due to the way the finite element formulation was reached, where the periodic boundary conditions were applied from outside the formulation through matrix operations, and not built into the formulation a priori, one is able to calculate the discrete Hamiltonian and overlap matrices from conventional finite element programs. The problem is then transformed into a standard complex-eigenvalue problem that is solved to calculate the energies of the system.

For a given finite element mesh, the results from the consistent and lumped overlap matrices were presented. The results from using a consistent overlap matrix provided an upper bound to the exact solution. On the other hand, the use of the lumped overlap matrix resulted, in most cases, in a lower energy value. A simple averaging procedure of the above two methods was performed. In general, this averaging process provided better results than both of the other two methods discussed above. Thus,

averaging may provide a method for improvement on the error without modifying the mesh.

REFERENCES

- [1] J. E. Pask, P. A. Sterne, "Finite element methods in *ab initio* electronic structure calculations," Modelling and Simulation in Materials Science and Engineering, vol. 13, pp. R71-R96, 2005.
- [2] J. E. Pask, B. M. Klein, P. A. Sterne and C. Y. Fong, "Finite-element methods in electronic-structure theory," Computer Physics Communications, vol. 135, pp. 1-34, 2001.
- [3] J. E. Pask, B. M. Klein and C. Y. Fong, "Real-space local polynomial basis for solid-state electronic-structure calculations: a finite-element approach," Physical Review B, vol. 59(19), 12352-12357, 1999.
- [4] N. Sukumar and J. E. Pask, "Classical and enriched finite element formulations for Bloch-periodic boundary conditions," International Journal for Numerical Methods in Engineering, vol. 77, pp. 1121-1138, 2009.
- [5] A. Leach, Molecular Modelling, Prentice Hall, 2001.
- [6] C. Metz, Physical Chemistry, Schaum's Outline Series, 1988.
- [7] O. Certik, J. Vackar and J. Plesek, "Density functional theory calculations using the finite element method," Proceedings of the Estonian Academy of Sciences, vol. 57(3), pp. 155-178, 2008.
- [8] J. Thijssen, Computational Physics, Cambridge University Press, 2007.
- [9] A. Wacker, An Introduction to the Concept of Band Structure, Lunds Universitet, 2010
- [10] J. N. Reddy, An Introduction to the Finite Element Method, McGraw-Hill, 2006.
- [11] M. Suzuki, I. Suzuki, Lecture Note on Solid State Physics, Bloch Theorem and Energy Band, 2006.