Periodic Numerical Grid Method for the Maximally Even Kronig-Penney Model

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Abstract

Energy band calculations for quasi-periodic crystals is an important field in condensed matter physics. Efficient and stable methods of calculation are necessary in the study of long quasi-periodic crystalline structures. The band gap structure of quasi-periodic crystals can be studied using a cell structure and applying a modified Kronig-Penney model. We show how a finite-element method using the discrete variable representation can be implemented with periodic boundary conditions on a Gauss-Lobatto Quadrature numerical grid. Because of the Gauss-Lobatto Quadrature numerical grid and the discrete variable representation, the local potential operators are represented as diagonal matrices and the kinetic energy matrix is quasi-block diagonal. This sparsity and block diagonal nature of the system greatly reduces the number of calculations necessary for the eigenvalue problem and increases the stability of the system as the size of the crystal chain grows. We implement the periodic finite-element discrete variable representation using a maximally even distribution of potentials as a modification to the usual Kronig-Penney model.

Introduction

Quasiperiodic and aperiodic single dimensional heterostructures constructed using mathematical chains such as the Fibonacci, Thieu-Morse and Cantor sets have lead to new technological applications in condensed matter (1; 2; 3). Other mathematical sets of interest in quasiperiodic one dimensional heterostructures include the Maximally Even sets (4) originally developed for studies in mathematical music theory. The Maximally Even set have been used to study the "devil's staircase" magnetic phases of spin=$1/2$ anti ferromagnetic systems(5) and also has been used in the study of ground state vortices in ladder arrays of Josephson junctions (5). These superlattice structures can be modeled as sequences of barriers and wells as originally done by Kronig and Penney (6)

The band spectra of the quasiperiodic and aperiod superlattice structures are important to the construction of these devices. Methods used to calculate the spectra of these superlattice structures include the spectral method (basis set expansion), numerical grid methods and the common transfer matrix method. With a continued increase in complexity in these superlattice structures the level of computational difficulty increases. Efforts to calculate the spectra of quasiperiodic superlattices using a discrete variable representation (DVR) have been done successfully by Rouzo (7) for the Kronig-Penney potential and Mathieu potentials. We propose an alternative method to solve the spectra problem by using a finite element method in conjunction with the DVR basis expansion, commonly known as FE-DVR, a technique proposed for quantum scattering problems by Rescigno *et al* (8). This finite element method greatly reduces the calculation size of a system and provides a stable Hamiltonian matrix which ensures accuracy in more complex superlattice structures.

Maximally Even Sets

The Maximally Even (ME) algorithm introduced by Clough and Douthett (4) is used to organize the sequence of barriers and wells of the Kronig-Penney model into a Maximally Even superlattice (5). An example of the 2 choose 1 barrier potential (note that the 2 choose 1 is just the Kronig-Penney model) and the 12 choose 5 barrier potential (also note that the 12 choose 5 set reproduces a 12 note musical octave(4)) is shown in figure 1. For a further discussion of the Maximally Even superlattices, please see poster **K1.0042** (5) in this conference.

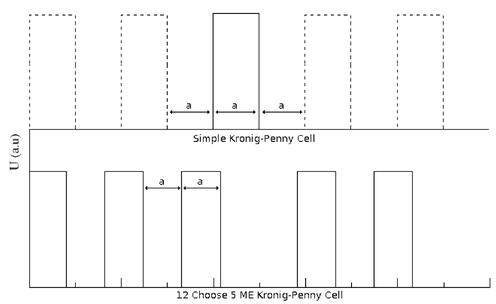

Figure 1. Potential energy examples

FE-DVR

A finite element (FE) method expands the wave function in terms of a collection of local operators spanning a grid of nodes $r_1 < r_2 < \cdots < r_N$ which replaces the independent variable r. Each local basis function $f_m^i(x)$ is defined to only span the interval $[r_i, r_{i+1}]$, and to be identically zero beyond each interval such that

$$f_m^i(x) = 0,\ \forall x \notin [r_i, r_{i+1}],\ i = 1, \cdots, N,\ m = 1, \cdots, n. \tag{1}$$

The index m is used to identify the local basis point, and used to implement the boundary conditions across each FE node. Furthermore the following conditions have to be satisfied:

$$f_1^i(r_i) = f_n^i(r_{i+1}) = 1, \tag{2}$$

$$f_m^i(r_i) = f_m^i(r_{i+1}) = 0 \text{ otherwise.} \tag{3}$$

Also to ensure that the wave function is continuous across each finite element node, the simple constraint that the wave function expansion coefficients c_m^i satisfy

$$c_n^i = c_1^{i+1} \tag{4}$$

Thus far no specification has been laid on the local basis function other than the boundary conditions listed in equations 2 and 3. In the DVR scheme, a polynomial is typically chosen to represent the local basis on diagonal matrices in conjunction with a Gaussian quadrature rule. This Gaussian quadrature rule is then used to calculate the overlap and Hamiltonian matrix elements. Any polynomial basis can be used to represent the local operators, examples include Hermite interpolating polynomials (9; 10), Jacobi polynomials (11) and Lagrange interpolating polynomials (12). We chose to use the Lagrange interpolating polynomials as our DVR basis in the same fashion as Manolopoulos and Wyatt (12) and Rescigno *et al* (8), such that

$$\begin{aligned} f_m^i(x) &= \prod_{\substack{j=1 \\ j\neq m}}^{n} \frac{(x - x_j^i)}{(x_m^i - x_j^i)},\ \ x \in [r_j, r_{j+1}] \\ &= 0,\ \ x \notin [r_j, r_{j+1}]. \end{aligned} \tag{5}$$

Also in the same mannor as Manolopoulos and Wyatt (12), the Gaussian quadrature rule is chosen to include the endpoints of each local basis interval. This is naturally done by choosing the Gauss-Lobatto quadrature method in which the weights w_m and points x_m are chosen such that the integral:

$$\int_{r_i}^{r_{i+1}} g(x)dx \cong g(r_i)w_1^i + \sum_{m=2}^{n-1} w_m^i g(x_m^i) + g(r_{i+1})w_n^i \tag{6}$$

is exact for polynomials of order $\leq 2n-1$. Across each DVR interval the Gauss-Lobatto weights and points are scaled as:

$$w_m^i = \frac{(r_{i+1} - r_i)}{2} w_m, \tag{7}$$

$$x_m^i = [(r_{i+1} - r_i)x_m + (r_{i+1} - r_i)]/2 \tag{8}$$

to correctly span each local basis interval.

The Lagrange interpolating polynomials (or as Manolopoulos and Wyatt (12) refer to them, Lobatto shape functions) satisfy equations 2 and 3 in that $f_m^i(x_{m'}^{i'}) = \delta_{i,i'}\delta_{m,m'}$. Furthermore the Lobatto shape functions are orthogonal under the Gauss-Lobatto quadrature rule such that

$$\int_0^\infty dx f_m^i(x) f_{m'}^{i'}(x) = \delta_{i,i'} \sum_j f_m^i(x_k^i) f_{m'}^i(x_k^i) = \delta_{i,i'}\delta_{m,m'} w_m^i. \tag{9}$$

Also note that all local operators have a diagonal representation

$$\int_0^\infty dx f_m^i(x) V(x) f_{m'}^{i'}(x) = \delta_{i,i'}\delta_{m,m'} w_m^i V(x_m^i). \tag{10}$$

To ensure continuity across each FE node, the Lobatto shape functions f_m^i and f_m^{i+1} are combined into a single bridge function defined as:

$$\chi_m^i(x) = \begin{cases} f_n^i(x) + f_1^{i+1}(x), & m = 1 \\ f_m^i(x) & m = 2, \ldots, n-1. \end{cases} \tag{11}$$

These bridge functions ensure continuity in the wave function across the FE intervals, and also give coupling between each finite element interval. Boundary conditions can then be applied by setting the first or the last bridge function to the desired value.

By expanding the wave function in terms of equation 11 and integrating by parts, the kinetic energy expectation value is found to be:

$$-\frac{1}{2}\int_0^\infty dx \psi(x) \frac{d^2}{dx^2}\psi(x) = -\frac{1}{2}\int_0^\infty dx \left(\frac{d}{dx}\psi(x)\right)^2. \tag{12}$$

Where the surface terms from the FE nodes cancel out after applying the boundary conditions given in equations 2, 3 and 4. By applying the Gauss-Lobatto integration rule to the right hand of equation 12, the kinetic energy matrix for this basis is readily found to be

$$\begin{aligned} T_{m,m'}^{i,i'} = \frac{1}{2}(\delta_{i,i'} + \delta_{i,i'\pm 1}) \int_0^\infty dx \frac{d}{dx}\chi_m^i(x) \frac{d}{dx}\chi_{m'}^{i'}(x) = \\ \frac{1}{2}(\delta_{i,i'} + \delta_{i,i'\pm 1}) \sum_k w_k^i \frac{d}{dx}\chi_m^i(x_k^i) \frac{d}{dx}\chi_{m'}^{i'}(x_k^i). \end{aligned} \tag{13}$$

It is important to note that the kinetic energy operator is completely dependent on the first derivative of the Lobatto shape function on the Gauss-Lobatto quadrature points, which is given by the equation

$$\frac{d}{dx}f_m^i(x_j^i) = \frac{1}{(x_m^i - x_j^i)} \prod_{k\neq m,j} \frac{(x_j^i - x_k^i)}{(x_m^i - x_k^i)} + \delta_{m,j} \sum_{k\neq j} \frac{1}{(x_m^i - x_k^i)}. \tag{14}$$

Thus the Hamiltonian matrix for the system will be given as

$$H_{m,m'}^{i,i'} = T_{m,m'}^{i,i'} + w_m^i V(x_m^i) I \tag{15}$$

where I is the NxN identity matrix.

Boundary conditions are implemented in the FE-DVR basis by simply setting the $H_{1,k}^{1,1}$ and $H_{k,1}^{1,1}$ or $H_{n,k}^{N,N}$ and $H_{k,n}^{N,N}$ elements (where $k = 1, \cdots, n$). In the case of collision calculations, where 0 boundary conditions are required, the desired endpoints are simply deleted from the basis. In the ME Kronig-Penney model we use the periodic boundary conditions

$$H_{n-k+1,n}^{N,N} = H_{k,1}^{N,N}, \text{ and } H_{n,n-k+1}^{N,N} = H_{1,k}^{N,N}, \text{ where again } k = 1, \cdots, n. \tag{16}$$

Numerical Work

We implement the Gauss-Lobatto quadrature by using the diagonalization algorithms presented by Golub *et al*(13; 14) and Stroud and Secrest(15) to solve for the quadrature rule weights and points. The resulting points and weights are scaled as shown by equations 7 and 8 and used in conjunction with equations 13 and 14 to calculate the Hamiltonian matrix $H_{m,m'}^{i,i'}$ given by eqn. 15. The LAPACK (16) linear algebra solving routines were used to solve the resulting eigenvalue problem to find the scaled spectra of the ME superlattice.

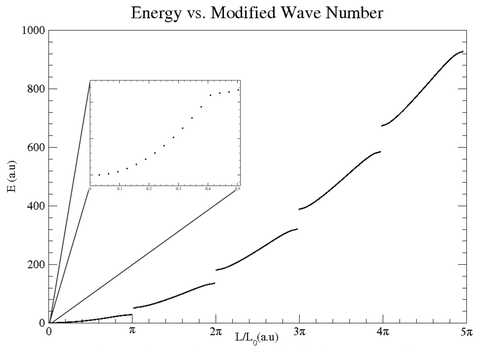

Figure 2. Five Kronig-Penney bands with low energy artifact

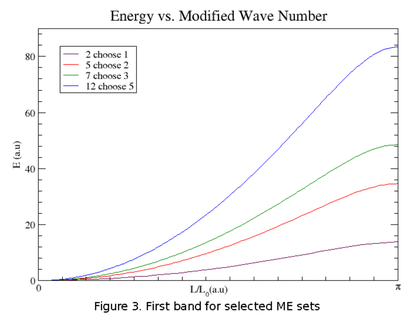

Figure 3. First band for selected ME sets

Discussion

The FE-DVR basis is attractive as a basis set for large scale problems over other DVR methods because while in both methods the number of nonzero Hamiltonian elements depend on the kinetic energy matrix, the FE-DVR basis scales as $(N-1)n^2 - N$ where the standard DVR basis scales as N^2. This significantly drops the number of elements that must be included in the eigenvalue problem and greatly improves the time required to run the calculation. Also the FE-DVR basis is practically useful in computational work because of how the finite element method alters the kinetic energy matrix from the standard DVR structure (a full NxN matrix) to a very sparse and structured matrix. Additionally, in the FE-DVR basis the kinetic energy matrix is represented as a strictly diagonally dominant, quasi-block diagonal matrix. Which further helps the problem by ensuring convergence of the eigenvalue problem.

Figures 2 and 3 show several calculated bands for the Kronig-Penney potential (figure 2) and a sequence of maximally even sets ranging from 2 choose 1 to 12 choose 6. In figure 2 we show that this method using the FE-DVR basis does indeed produce the correct band structure for the Kronig-Penney model. As can be seen in the subplot of figure 2, there is a small L/L_0 artifact in the energies which corresponds to the limit where the Kronig-Penney cell goes to zero. This is an expected phenomena based on the non-standard method used for solving for the Kronig-Penney spectrum. Because the FE-DVR basis has shown the potential to produce the correct band structure, future work will have to involve solving for the correction factor to transform the spectrum produced here to the standard Kronig-Penney form.

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