Abstract

Energy band calculations for quasi-periodic crystals is important in both condensed matter physics. Efficiently calculating electron wave functions and obtaining a correct band structure is a central problem in computational solid-state physics. Within this framework lies the Kronig-Penney model, which is a one-dimensional Kronig-Penney model with periodic boundary conditions. The Hamiltonian matrix is a quasi-block diagonal matrix, which greatly reduces the number of elements that must be included in the eigenvalue problem and greatly improves the time required to run the calculation. The FE-DVR basis is practical in computational work because of its efficiency. The finite element method further helps the problem by ensuring convergence of the eigenvalue problem.

Introduction

Quasiperiodic and aperiodic single-dimensional heterostructures constructed using mathematical structures such as the Fibonacci, Thue-Morse and Cantor sets have lead to new technological applications in condensed matter physics including the Maximally Even sets (4) originally developed for studies in mathematical music theory. The Maximally Even set have been used in 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 DVR basis. In the ME Kronig-Penney model we use the periodic boundary conditions and use the DVR basis in the same fashion as Manolopoulos and Wyatt (12) and Rescigno (8), such that the integral

\[ \int_{-\infty}^{\infty} \psi_i(x) \psi_j^*(x) dx = \delta_{ij} \]

is exactly polynomials of order \( \leq 2 \). Across each DVR interval the Gibbs-Lobatto weights and points are scaled as:

\[ \alpha_i = \frac{\alpha_{i+1}}{\alpha_{i-1}} + \frac{\alpha_{i-1} - \alpha_{i+1}}{2\alpha_{i-1}} \]

allowing the calculation of a symmetric FE-DVR basis. 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. The FE-DVR basis is practical in computational work because of its efficiency. The finite element method further helps the problem by ensuring convergence of the eigenvalue problem.

Maximally Even Sets

The Maximally Even (ME) algorithm introduced by Clough and Duff (13) is used to generate a sequence of bases for an n-dimensional model into a Maximally Even superstructure (5). An example of the 2-dimensional 1x2 periodic potential made from the Kronig-Penney model is shown in figure 1. For a further discussion of the Maximally Even superstructure, please see project K1.0042. In this conference we implement the periodic finite-element method to solve the Kronig-Penney model and compare numerical results with equation 12, the kinetic energy matrix for this basis is readily found to be

\[ H = \begin{pmatrix} 
1 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 \\
0 & 0 & 1 & 1 
\end{pmatrix} \]

This confirms the diagonal nature of the system as the size of the crystal chain grows. We implement the periodic finite-element method to solve the Kronig-Penney model and compare numerical results with equation 12, the kinetic energy matrix for this basis is readily found to be

\[ H = \begin{pmatrix} 
1 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 \\
0 & 0 & 1 & 1 
\end{pmatrix} \]

FE-DVR

A finite element (FE) method expands the wave function in terms of a collection of local operators spanning a product Hilbert space \( \psi(x) = \sum_{i} \psi_i \chi_i(x) \)

with the indices \( \{ i \} \) representing the independent variable \( x \). Each local basis function \( \psi_i(x) \) is defined to only span the interval \( x_i \leq x < x_{i+1} \), and to be identically zero beyond each interval such that

\[ \int_{-\infty}^{\infty} \psi_i(x) \psi_j^*(x) dx = \delta_{ij} \]

The index \( i \) 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:

\[ f_i(x) = \frac{f_i(x_{i+1}) - f_i(x_i)}{x_{i+1} - x_i} \]

Also to ensure that the wave function is continuous across each finite element node, the simple constraints that the wave function expansion coefficients \( c_i \) satisfy

\[ c_i = c_i' \]

are used. This for sure specifies how fast the local basis function itself the boundary conditions are satisfied in equation 2 and 3. 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 matrices, which are polynomial matrices which can be represented by local operators, simple basis interpolating polynomials (9, 10), finite polynomials (11) and Lagrange interpolating polynomials (12). We choose to use the Lagrange interpolating polynomials as our DVR basis in the same basis as Manolopoulos and Wyatt (12) and Rescigno (8), such that

\[ f_i(x) = \frac{\prod_{k \neq i} (x - x_k)}{\prod_{k \neq i} (x_i - x_k)} \]

Also in the same manner as Manolopoulos and Wyatt (12), the Gaussian quadrature rule is chosen to include the elements of each local basis interval. This is naturally done by choosing the Gaussian quadrature points to number of points \( n_l \) on the interval \( x_i \leq x < x_{i+1} \), which are chosen such that the integral

\[ \int_{x_i}^{x_{i+1}} \psi_i(x) \psi_j^*(x) dx = \frac{\alpha_{i+1}}{\alpha_i} \delta_{ij} \]

is exactly polynomials of order \( \leq 2 \). Across each DVR interval the Gibbs-Lobatto weights and points are scaled as:

\[ \alpha_i = \frac{\alpha_{i+1}}{\alpha_{i-1}} + \frac{\alpha_{i-1} - \alpha_{i+1}}{2\alpha_{i-1}} \]

where \( i, j = 1, 2 \). 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. The FE-DVR basis is practical in computational work because of its efficiency. The finite element method further helps the problem by ensuring convergence of the eigenvalue problem.

Numerical Work

We implement the Kronig-Penney model by using the diagonalization algorithm presented by Gehrke et al. (6), Hur and Schouten (7) to solve for the quadrature weights and points. The resulting weights and points are scaled as shown by equations 7 and 8 and used in conjunction with equations 9 and 10 to calculate the Hamiltonian matrices, expressed given by equation 15. The LAPACK (16) linear algebraic-solving routines were used to solve the eigenvalue problem for the scaled operator of the ME superstructure.

\[ H = \begin{pmatrix} 
1 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 \\
0 & 0 & 1 & 1 
\end{pmatrix} \]

Energy vs. Modified Wave Number

Discussion

The FE-DVR basis is attractive as a basis set for large-scale problems over DVR methods. Because in both DVR methods the number of nodes associated with the kinetic energy matrix, the FE-DVR basis scales as \( N \cdot N \), 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 its efficiency. The finite element method alters the kinetic energy matrix from the standard DVR structure (17) \( N \cdot N \) matrix to a very sparse and unique 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 (2) and a Magnus and numerically exact wave matrix (21) to (23) in figure 2 and 3. In figure 3 we show that this method using the FE-DVR basis does indeed produce the correct band structure for these superlattice models. As can be seen in the figures of 2 and 3, there is a small 5x5 artifact in the energies which corresponds to the finite size 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, we now look for methods to scale solving for the eigenvalue problem to the size of the periodic boundary conditions.

References


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Figure 1. Potential energy examples

Figure 2. 2D Kronig-Penney band and lines with line energy artifact

Figure 3. Print band for selected HSE sets

Figure 4. First Kronig-Penney bands with low energy artifact

Figure 5. Kronig-Penney bands with low energy artifact