Computing the Density of States and Energy Bands of a 1-Dimensional Lattice Using Transfer Matrices

P.T. Galwaduge

Department of Physics

Drexel University

The Kronig-Penney model is typically used to compute the band structure and bound states of a periodic crystal. While the model allows analytical solutions, it does so by simplifying the potential to a periodic square potential. We present a method of using transfer matrices to compute energy bands in a 1-Dimensional lattice. This method does not involve the simplification required by the Kronig-Penney model and has the advantage of being able to model 'real' potentials.

I. Introduction

Solid-state systems are inherently quantum mechanical in nature. Despite their ubiquitousness, only a small number of quantum mechanical problems are analytically tractable. Because of this, it is common to use simplifications and perturbative approaches when solving complex problems. Kronig-Penney model is an example of such a simplified approach to solving a quantum mechanical problem. The model replaces the lattice with a series of equidistant square well potentials or delta functions[1]. Square wells and delta function potentials have known analytical solutions. Hence, by applying this model and applying Bloch functions, it is possible to compute the band structure and the density of states of a periodic lattice[2]. Potentials encountered in nature rarely take the form of square wells or delta functions. This is a shortcoming of the model.

We propose to overcome this shortcoming by using an alternative approach of calculating the band structure and density of states. The technique, which involves the use of transfer matrices solves for the potential piece by piece. First, we shall develop the technique for a square well potential as described in ref [3]. We will later discuss how the technique can be used to model potentials other than square wells and finally present results of applying the technique to a 1-dimensional lattice with a two atom unit cell.

II. A Matrix Approach to Solving Piecewise Potentials

Piecewise potentials can be tedious to solve analytically. However, given the repetetive nature of the process, computers can be utilized to solve these with ease. Representing the problem in terms of matrices simplifies computer representation of the problem. The following section discusses a matrix based approach to solving piecewise potentials.

Matrix Representation of a Single Well Problem

Consider a series of potential wells. The general form of the wave function is given by,

$$\Phi(x) = A_j\Phi_1(x) + B_j\Phi_2(x) \tag{1}$$

with Φ_1 and Φ_2 representing the solution to the time independent Schrödinger equation in region j. Note that the exact form of Φ_1 and Φ_2 depends on the relation between E and V. For E > V and E < V, the solutions are in the form of plane waves.

The relation between the coefficients A_j and B_j can be expressed in terms of matrix notation. We will start by considering a potential consisting of just one square well. The relation between the left hand side of the well and the right hand side of the well, which we shall denote as regions 1 and 2 respectively, are given by:

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = T_{12} \begin{bmatrix} A_2 \\ B_2 \end{bmatrix} \tag{2}$$

ref [3]

T_{12} is the transfer matrix relating the two sides of the potential. It is given by:

$$T_{12} = E^{-1}(V_1; a_1)K^{-1}(V_1)K(V_2)E(V_2; a_2) \tag{3}$$

where,

$$E(V, x) = \begin{cases} \begin{bmatrix} e^{ikx} & 0 \\ 0 & e^{-ikx} \end{bmatrix}, E > V \\ \begin{bmatrix} 1 & x \\ 0 & 1 \end{bmatrix}, E = V \\ \begin{bmatrix} e^{-\kappa x} & 0 \\ 0 & e^{\kappa x} \end{bmatrix}, E < V \end{cases} \tag{4}$$

$$K(V) = \begin{cases} \begin{bmatrix} 1 & 1 \\ +ik & -ik \end{bmatrix}, E > V \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, E = V \\ \begin{bmatrix} 1 & 1 \\ -\kappa & +\kappa \end{bmatrix}, E < V \end{cases} \qquad (5)$$

ref [3]

with $k = \sqrt{2m(E - V)/\hbar^2}$ and $\kappa = \sqrt{2m(V - E)/\hbar^2}$. Note that the above is simply the solutions to the time independent Schrödinger equation expressed in matrix form.

Matrix Representation of Multiple Wells

For multiple potential wells, each well can be treated as a new problem. The problem can be solved piece by piece from left to right. Matrix representation can make the process of solving mutiple well problems elegantly simple. It is possible to write down a general expression for a transfer matrix $T_{j,j+1}$ which relates region j to region j+1:

$$T_{j,j+1} = E^{-1}(V_j; a_j)K^{-1}(V_j)K(V_{j+1})E(V_{j+1}; a_j) \qquad (6)$$

ref [3]

A transfer matrix for the whole set of potetials can be generated by multiplying transfer matrices representing each piece of the potential. Multiplication of the transfer matrices leads to the following expression:

$$\begin{bmatrix} A'_L \\ B'_L \end{bmatrix} = T_{L,R} \cdot \begin{bmatrix} A'_R \\ B'_R \end{bmatrix} \qquad (7)$$

ref [3]

$T_{L,R}$ is the transfer matrix relating the asymptotic left hand and the asymptotic right hand regions.It is given by:

$$T_{L,R} = K^{-1}(V_L) \cdot M \cdot K(V_R) \qquad (8)$$

ref [3]

A'_L and B'_L represent amplitudes in the asymptotic left hand reigion. They have been formed by absorbing $E(V_L; a_0)$ into the amplitudes A_L and B_L. Similarly A'_R and B'_R are amplitudes representing the asymptotic right hand region. They have been formed by absorbing $E(V_R; a_n)$ into the amplitudes A_R and B_R. Matrices $K^{-1}(V_L)$ and $K(V_R)$ represent the asymptotic left hand and right hand regions.

For a potential with n pieces with the boundaries of the pieces occuring at a_j:

$$M = \prod_{j=1}^{n} M(V_j, \delta_j) \qquad (9)$$

$$M(V_j, \delta_j) = K(V_j)E(V_j; a_{j-1})E^{-1}(V_j; a_j)K^{-1}(V_j) \qquad (10)$$

ref [3]

With $\delta_j = a_j - a_{j-1}$. Thus, we have demonstrated a technique of solving the time independent Schrödinger equation across a piecewise potential comprising of square wells.

Modeling Real Potentials

The earlier section dealt exclusively with square wel potentials. While using the transfer matrix approach has made computation simple, the technique was developed for square well potentials. However, the technique can be extended to solve other potentials. It is possible to represent smooth potentials such as Gaussians, in terms of a series of square well potentials. The number of wells used to represent the potential can be increased until the desired smoothness is achieved. This idea will be revisited in the results section.

Periodic Boundary Conditions

Since our interest lies in lattices, we now apply periodic boundary conditions to the above formulation. We will consider a periodic potential with N potentials. As discussed before, the transfer matrix will relate the amplitudes of two consecutive pieces:

$$\begin{pmatrix} A \\ B \end{pmatrix}_i = T \begin{pmatrix} A \\ B \end{pmatrix}_{i+1} \qquad (11)$$

Since the potential consists of N pieces,

$$\begin{pmatrix} A \\ B \end{pmatrix}_i = T^N \begin{pmatrix} A \\ B \end{pmatrix}_{i+N} \qquad (12)$$

Periodicity requires that the wavefunction at the ith piece and (N+i)th have to match. Thus:

$$\begin{pmatrix} A \\ B \end{pmatrix}_i = \begin{pmatrix} A \\ B \end{pmatrix}_{i+N} \qquad (13)$$

which implies that,

$$T^N = I_2 \qquad (14)$$

ref [3]

Where I_2 is the 2x2 unit matrix. By applying the similiarity transformation mentioned in ref [3] (pp. 168) and chossing matrix S to diagonalize T, eigenvalues can be computed in terms of a single unit cell transfer matrix. The eigenvalue equation is then given by:

$$det\left[\begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} - \lambda I_2 \right] = 0 \qquad (15)$$

simplification yields:

$$\lambda_\pm = \frac{1}{2}tr(T) \pm i\sqrt{1 - (\frac{1}{2}tr(T))^2} \qquad (16)$$

When $|\frac{1}{2}tr(T)| \leq 1$ define angle ϕ such that:

$$cos\phi = \frac{1}{2}tr(T) \qquad (17)$$

Then the eigenvalues of the transfer matrix are given by:

$$\lambda_{\pm}(E) = e^{\pm i\phi(E)} \qquad (18)$$

Note the quantization condition is $cos\phi(E) = \frac{1}{2}tr(T(E))$ and $\Phi = \frac{2\pi k}{N}$.

ref [3]

Density of States

The density of states $\rho(E)$ gives the number of states within an energy range ΔE which contains the energy E. The angular difference $\Delta\Phi$ is proportional to the number if states in the interval ΔE. Each energy band will contain N states. Thus:

$$\frac{dN}{N} = \frac{\rho(E)dE}{N} = \frac{d\Phi}{dE} \qquad (19)$$

$$\rho(E) = \frac{N}{2\pi}\frac{d\Phi}{dE} \qquad (20)$$

Since we are using a computational approach, the density of states can be estimated as the difference of Φ over an energy step.

$$\rho(E) \sim \Phi(E_{i+1}) - \Phi(E_i) \qquad (21)$$

ref [3]

Algorithm

For clarity, we now restate the algorithm for computing energy bands and the density of states given in ref [3]:

1. Choose a value of E.
2. Compute $M(V_i; \delta_j)$ for each piece of the potential in the unit cell using equation (10).
3. Compute the transfer matrix for the unit cell by mutiplying in order, all the matrices computed in the previous step.
4. Compute $cos(\phi)$ as described in equation (17).
5. Compute ϕ for cases where $|cos(\phi)| \leq 1$.
6. Construct the density of states plot using equation (21).
7. Construct the energy band plot using the computed values of ϕ.

III. Results

Now we present the band structure and density of state calculations performed using the method described above. The computation was was implemented on MAPLE 12. All calculations were performed with an energy resolution of 0.001 eV. Each computation was completed within a matter of minutes on a standard computer.

Unit Cell With Two Atoms

We attempt to apply the above technique to compute the band structure and density of states of a 1-dimensional lattice consisting of a two atom unit cell. We assume the real potential of the unit cell is in the form of a dual gaussian as shown below:
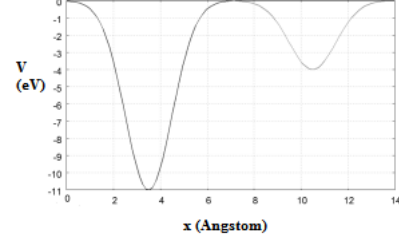

Figure 1. Potential of a two atom unit cell

Approximation with Two Square Potentials. Now we approximate the above potential with two square wells as seen in the figure below, so that the unit cell is approximated by 4 pieces.
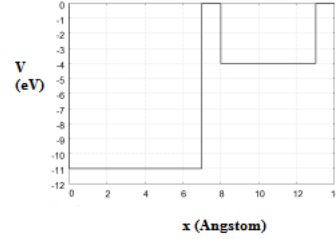

Figure 2. Dual square well approximation of the dual gaussian potential

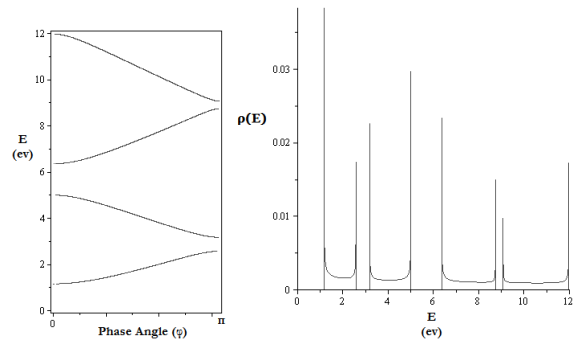The computation results in the following:

Figure 3. Energy Bands(Left) and Density of States(Right) of the potential approximated by two square wells

Some of the energy band lines do not extend all the way from 0 to π. This is an artifacact of the energy resolution and can be resolved by choosing a smaller energy step in the calculation.

Gaussians Approximated With Many Square Wells. We now repeat the above computation. In this case, the two

gaussians have been approximated with seven piece and five piece square well potentials respectively, so that the unit cell is approximated by 14 pieces. The figure below shows the potential approximation:
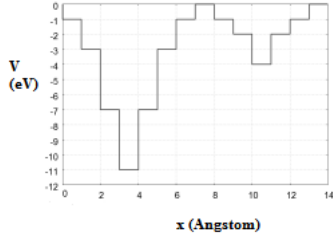

Figure 4.   Gaussians approximated by 14 pieces

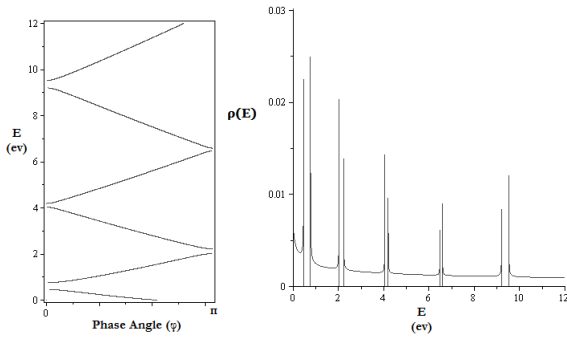The results of the computation are as follows:

Figure 5.   Band Structure(Left) and Density of States(Right) for the potential approximated by 14 pieces

Discussion

There is a clear difference between the energy bands computed using the two different approximations given above. The two well approximation gives energy bands which are clearly seperated. In the case of the 14 piece approximation, the energy band gaps become smaller. This suggests that using simple approximations might yield results that are not fully representative of the original system under study. While the approximations we made involved hard potentials, the number of potential pieces can be easily increased until they represents a smooth gaussian.

We have presented a technique of computing the band structure and density of states of a 1-dimensional lattice. The method does not require the extreme simplification required by the Kronig-Penney model but maintains the computational simplicity of solving the Schrodinger equation for potential wells. The technique can be easily implemented on a computer. The main strength of the technique is its ability to model smooth potentials, thus being able to model potentials that occur in nature.

References

1. L. Kronig, R. de, & Penney, W. G. (1931).   *Quantum mechanics of electrons in crystal lattices. Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character*, 130, 499-513.

2. Kittel, C. (2005). *Solid state physics*. Wiley.

3. Gilmore, R. (2004).   *Elementary quantum mechanics in one dimension*. Johns Hopkins University Press.