Numerical Matrix Method for Kronig-Penney Model for Periodic Potential

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Abstract—The project aims to compute energy eigenvalues of Periodic Potential. The computation was done by forming the Hamiltonian Matrix of the desired Periodic Potential and finding its eigenvalues and, thence, the allowed energy eigenvalues. The results were compared with the analytical solutions of the Konig-Penny Model for Periodic Potentials. Further, the effect of the external electric field applied to this system was investigated, and the variation in energy eigenvalues and bandgaps was recorded.

Index Terms—Periodic Potential, Konig-Penney Model, Energy-Band diagrams, Numerical Solutions

1 Introduction

THIS project studies the Numerical Matrix Metod to compute energy eigenvalues for any general Hamiltonian. The aim is to study the merits and drawbacks of this method. We will briefly illustrate the mathematical background of the model and try to implement the same for a Periodic Potential Model.

2 THE MATRIX METHOD

To solve the Schrodinger Equation for a generalised case, we first have to choose a basis set of wavefunctions that forms a complete basis. The simplest set that comes to mind in an Infinite Potential Well. The Hamiltonian corresponding to the same is:

$$H_o = \frac{\hat{p}^2}{2m} + V_{inf} \tag{1}$$

$$H_o u_i = E_i^0 u_i \tag{2}$$

where,

$$V_{inf}(x) = \begin{cases} 0 & x \in (0, L) \\ \infty & otherwise \end{cases} \tag{3}$$

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Let an arbitrary potential $V(X)$ be superimposed over V_{inf}. We take the width of V_{inf} to be large enough such that $V(x)$ mimics its ideal case. Thus, we have to solve the eigenvalue equation for,

$$H\left|\psi\right\rangle = E\left|\psi\right\rangle \tag{4}$$

where,

$$H = H_o + V(x) \tag{5}$$

Since the energy eigenfunction of Infinite Potential forms a complete basis set, we can write

$$\left|\psi\right\rangle = \sum_{i=1}^{\infty} c_i \left|u_i\right\rangle \tag{6}$$

Substituting in 3,

$$H\sum_{i=1}^{\infty} c_i \left|u_i\right\rangle = E\sum_{i=1}^{\infty} c_i \left|u_i\right\rangle \tag{7}$$

Taking inner products with $\langle u_j|$,

$$\sum_{i=1}^{\infty} c_i H_{ij} = E c_j \tag{8}$$

where,

$$H_{ij} = \langle u_j|H|u_i\rangle = \delta_{ij}E_i^0 + \frac{2}{L}\int_0^L sin(\frac{i\pi x}{L})V(x)sin(\frac{j\pi x}{L})dx \tag{9}$$

The above result is true for any general $V(x)$ given $V_{inf}(x)$ is wide enough. Equation 8 is an infinite dimension Matrix Eigenvalue Equation. For computational purposes, we can truncate

it to a finite value and find the Eigenvalues and corresponding Eigenvector, which can be substituted back in 6 to get the Energy Eigenfunction of H. It can be seen that $H_{ij} = H_{ji}$, i.e., the H matrix is symmetric. This result can be used to calculate the H matrix faster.

3 KONIG-PENNEY MODEL

3.1 Description

We consider a one-dimension lattice where the Lattice constant a=1, and potential barrier width=1/16. We take n_b such barrier equally spaces.

$$V_{KP}(x) = \begin{cases} V_o, & |x - x_r| < \frac{b}{2} \\ 0, & otherwise \end{cases} \tag{10}$$

where $x_r = -a/2 + ra$ is the location of r^{th}barrier, $r \in \{1, 2, ..., n_b\}$.

For our computation we used n_b={10,20,30} and N (dimension of matrix) to be {150,600}. These values provided minimum deviation of results from the analytical model.

For the second part of the problem, the superimposed potential was of the form:

$$V_{KP2}(x) = V_{KP}(x) + \epsilon x \tag{11}$$

We vary ϵ to increase the exterior field strength.

3.2 Computational Results

The plots were made to compare the energy eigenvalue of Infinite Potential Well, and the numerical and analytical results of KP-Model. The analytical model is described later in the report. Figure 1 is computed for n_b=10, N=150; the remaining parameters remain the same. Figure 2 is computed for n_b=10, N=150; the remaining parameters remain the same. While computation you can observe some negative values, which can be discarded since the allowed energies are strictly positive. The values are merely possible mathematical solutions to Eigen-equation but don't hold physically.

We can see three bands of allowed energy and two forbidden regions where no energy is allowed for real values of k. The first energy band gap computed for both figures is 10.48 and 10.07 units, respectively. It can be observed that on increasing n_b, we get more accurate energy eigenvalues and hence the measure of the band gaps. Also, more points are available, which is good if some interpolation is used to find other values.

On increasing n_b to 30, we get accurate results in the third band too. The value of N does not play much significance as long as it is very large (5-6 times) than n_b. Using a larger N gives us more energy eigenvalues without much change in the accuracy of those values. Figure 3 shows computation for n_b=20 and N=600.

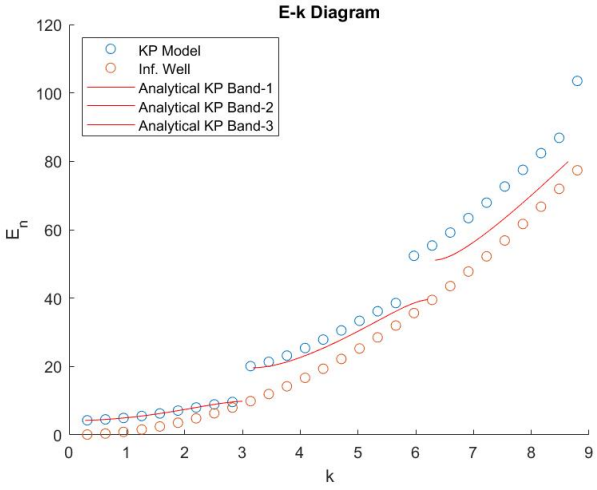

Figure 1. Energy Eigenvalues. n_b=10, N=150

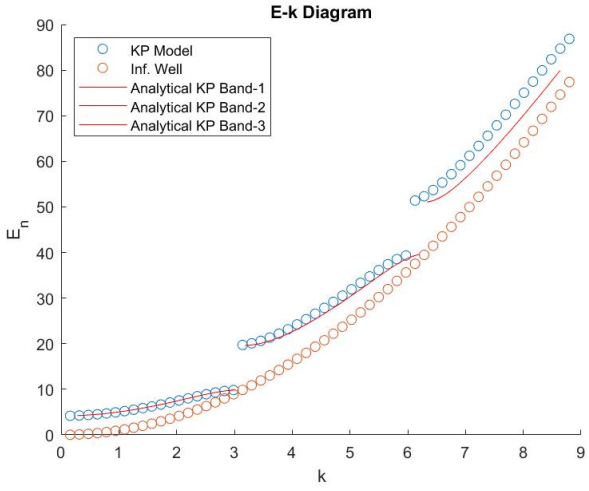

Figure 2. Energy Eigenvalues. n_b=20, N=150

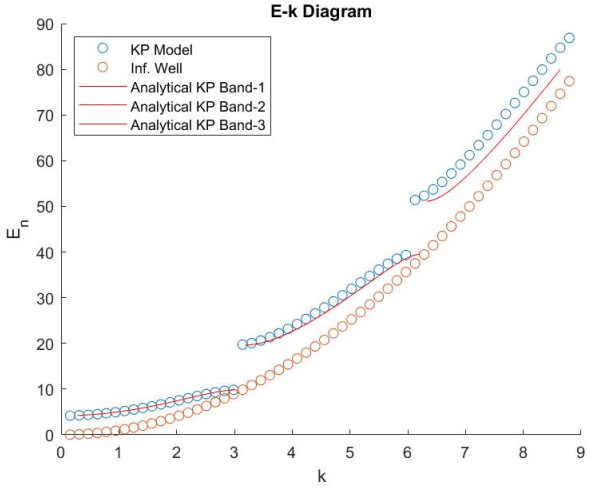

Figure 3. Energy Eigenvalues. n_b=20, N=600

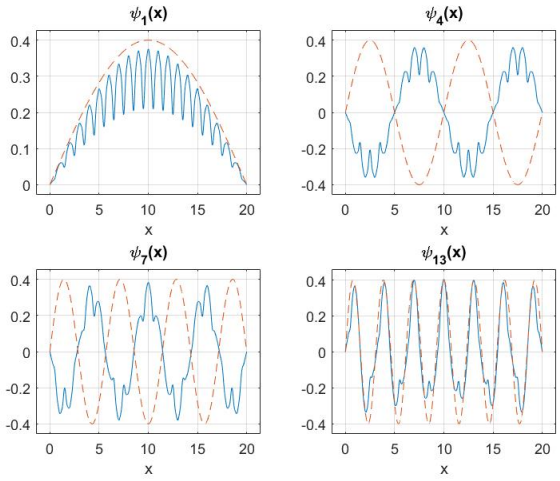

Figure 5. Eigenstates n_b=20, N=150

The corresponding wavefunctions have been plotted too. An important observation is the n^{th} eigenfunction of the KP model has a similar shape to the n^{th} eigenfunction of Infinite Potential Well. This is even verified numerically as for the n^{th} eigenfunction $c_n >> c_j$ when $j \neq n$.

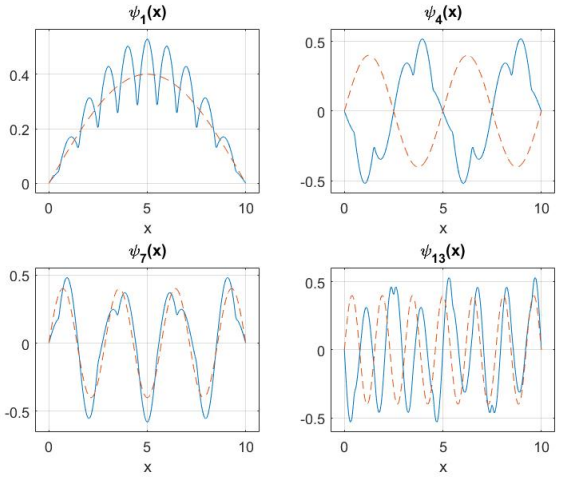

Figure 4. Eigenstates n_b=10, N=150

3.3 Computational Results: External Field

The potential used to study the impact of external electric field on the system was modelled along the lines of Equation 11 where $\epsilon \in \{0, 0.1, 0.8, 2\}$. Figure 6 shows the energy eigenvalues and figure 7 shows $\psi_1(x)$ for all ϵ.

It can be seen that as the electric field increases (increase in ϵ), the band gap decreases. For $\epsilon = 2$, the bandgap completely diminishes, and we get a continuous band of energies.

Correspondingly, the wavefunctions also shift towards $x = 0$ with increasing. Consequently, the probability of finding an electron in its first eigenstate increases in the region closer to $x = 0$. One should note that the change in $\psi_1(x)$ is very large for even a minimal change in ϵ. The energy bands hardly change for such small ϵ.

Devices that take advantage of the band gaps (lasers, diodes, etc.) can be fine-tuned as per our requirement by application of such external fields, and the lattice structure does not constrain us.

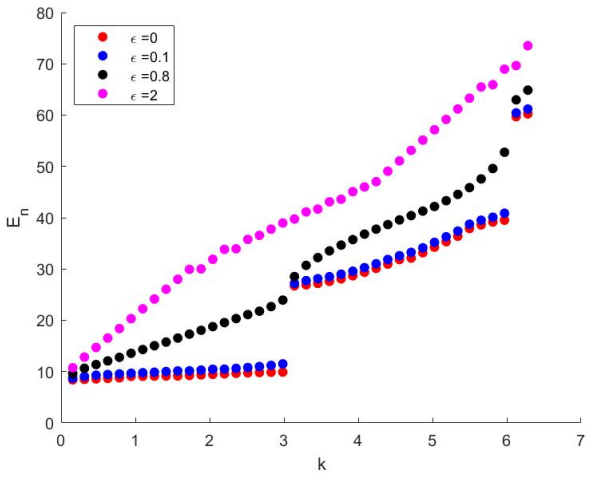

Figure 6. Eigenstates n_b=20, N=150

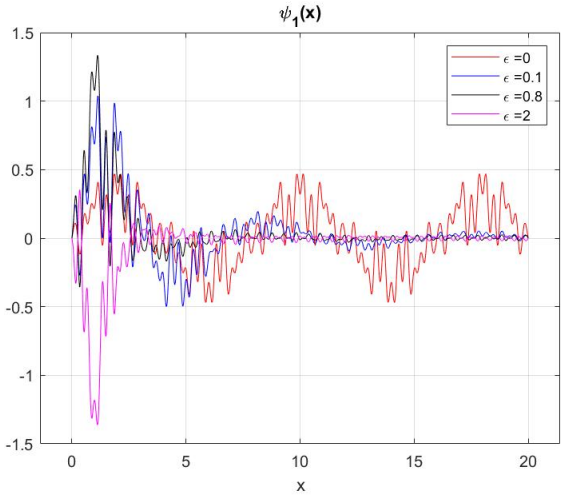

Figure 7. Eigenstates n_b=20, N=150

4 Analytical KP Model

Schrodinger's Equation for V=0 and V=V_0 can be respectively written as,

$$\frac{\partial^2\psi}{\partial x^2} + \alpha^2\psi = 0; \alpha^2 = \frac{2mE}{\hbar^2} \tag{12}$$

$$\frac{\partial^2\psi}{\partial x^2} - \beta^2\psi = 0; \beta^2 = \frac{2m(V_0 - E)}{\hbar^2} \tag{13}$$

The solution for the above partial differential equation takes the form

$$\psi_1(x) = A\sin\alpha x + B\cos\alpha x \tag{14}$$

$$\psi_2(x) = C\sinh\alpha x + D\cosh\alpha x \tag{15}$$

On applying boundary conditions and using Bloch's Theorem, we get the following constraint equation for (A,B,C,D) to have a non-trivial solution.

$$\cos(ka) = \frac{\beta^2 - \alpha^2}{2\alpha\beta}\sinh(\beta b)\sin(\alpha(a-b)) + \cosh(\beta b)\cos(\alpha(a-b)) \tag{16}$$

For limiting case (as in our example), $V_0 >> 1$ and $b << 1$, the above equation can be re-written as,

$$P\frac{\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka \qquad P = \frac{mV_0ab}{\hbar^2} \tag{17}$$

In17, the LHS is a function of α, which stores the information about E. When —LHS—¿1, the equation will yield no real solutions for k. Plotting LHS, we get 8

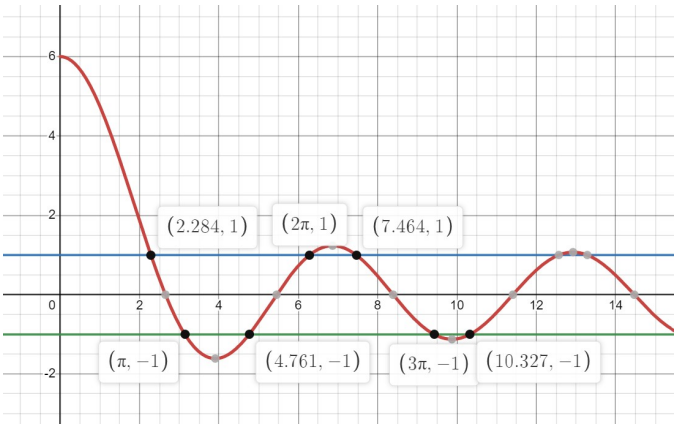

Figure 8. $y = 5\frac{\sin\alpha a}{\alpha a} + \cos\alpha a$

We can see for certain values of α, we will get no real solution for k. These values of α, and in turn of E, form the forbidden band of energies we observed in our computations.

5 Conclusions

The Matrix Method provides a fast method to compute numerical energy eigenvalue and eigenstate for any random potential field. Further, studying effects of external potentials and fields on the system can also be studied effectively using this system. We looked at the numerical solutions of Konig-Penny Model, which were further compared with the analytical solution. The numerical solution had minimum deviation from analytical models thereby reinforcing the effectiveness of the Numerical Matrix Method.