PH3203: Advanced Quantum Mechanics
Spring'24

Determination of 1D band structure by transfer matrix method

Abstract

We have reproduced the result of [2] and have numerically shown that the discretized form of the Schrodinger and Dirac equation for a smooth potential in one dimension is equivalent to Poincare map of the corresponding wave equation for an array of $\delta-$function potential(in each cell we have an array of $\delta-$function with weight factor determined by the potential that we are studying). We can map a general periodic potential to a generalized Kronig-Penney model to study the dynamics of electrons in the lattice. The transfer matrix method is used to compute the energy band and dispersion relation. We have used this method to calculate the band structure of a cosine background potential for both non-relativistic and relativistic cases.

Soudip Kundu
21MS051
sk21ms051@iiserkol.ac.in

Krishnabh D. Nandy
21MS226
kdn21ms226@iiserkol.ac.in

Rohan Kumar
21MS019
rk21ms019@iiserkol.ac.in

Contents

1 Introduction

One-dimensional models are important in understanding the behavior of electrons in lattices. this model helps us understand important concepts like block states, energy bands, and gaps. we generally use an array of square wells or $\delta-$function potentials(Kronig and Penny) which is a crude picture of the electron interaction with other electrons and atoms in a solid. numerical solutions of the wave equation corresponding to a general potential give accurate results where analytical solutions are absent. discretization of the Schrodinger and Dirac equation is widely used in the numerical solution for calculating one-dimensional bands.

This paper reproduces the result of [2] where they use an alternate numerical method to study the dynamics of non-relativistic and relativistic electrons in one-dimensional potentials. The discretized forms of the Schrodinger and Dirac equations can be replaced by the Poincare map associated with the corresponding wave equation for an array of $\delta-$function potential. We have also shown that the error for both the process Poincare map approach and the original discretization scheme are almost similar. For a general periodic potential, we can map the problem to the generalized Kronig-Penney or the Dirac-Kronig-Penney model with the same period. This replacement will allow us to use the transfer matrix technique for computing the dispersion relation. Numerical results are provided under the section Numerical Analysis. The convergence of these methods(analytical solution and generalized Kronig Penney solution) is shown with the help of an example and non-relativistic and relativistic band structures are compared.

2 General Proof of Bloch's Theorem

Consider a 1D periodic potential where $V(x \pm a) = V(x)$, as shown in the figure. In reality, we may consider the motion of an electron in a chain of regularly spaced positive ions. Let us define a translation operator $\tau(a) = e^{\frac{iPa}{\hbar}}$ whose properties are

$$\tau(a)\left|x\right\rangle = \left|x+a\right\rangle, \qquad \tau(a)^{\dagger} x \tau(a) = x + a$$

Now, as a is the lattice spacing, we can write

$$\tau(a)^{\dagger} V(x) \tau(a) = V(x+a) = V(x)$$

Now let us take our Hamiltonian to be $\hat{H} = \frac{P^2}{2m} + V(x)$ and check if its invariant under the translation

$$\begin{aligned}
[\tau(a), \hat{H}] &= [\tau(a), \frac{P^2}{2m}] + [\tau(a), V(x)] \\
&= [\tau(a), V(x)] \\
&= \tau(a)V(x) - V(x)\tau(a) \\
&= V(x+a) - [\tau(a)^\dagger V(x)]^\dagger \\
&= V(x+a) - [V(x-a)]^\dagger \\
&= 0
\end{aligned}$$

Thus, we see that the Hamiltonian is invariant under the translation operator. The entire Hamiltonian satisfies,

$$\tau(a)^\dagger \hat{H} \tau(a) = \hat{H}$$

Because $\tau(a)$ is unitary. So, the Hamiltonian and $\tau(a)$ can be simultaneously diagonalized. Although $\tau(a)$ is unitary, it is not Hermitian, so we expect the eigenvalue to be a complex of modulus 1.

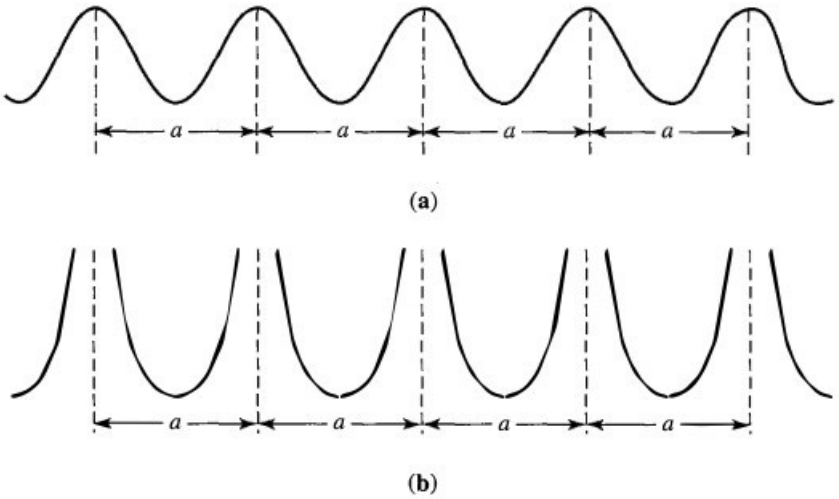


Figure 1: (a) Periodic potential in one dimension with periodicity a. (b) The periodic potential when the barrier height between two adjacent lattice sites becomes infinite

Now consider $|n\rangle$ (a particle localized in a n^{th} state), which is an eigenstate of the Hamiltonian.

$$\hat{H} |n\rangle = E_0 |n\rangle$$

$$\tau(a) |n\rangle = |n+1\rangle$$

but not an eigenstate of the translation operator. We aim to find a simultaneous eigenket of $\hat{H}$ and $\tau(a)$. Let us specifically form a linear combination.

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta} |n\rangle$$

where θ is a real parameter with $-\pi < \theta < \pi$. We assert that $|\theta\rangle$ is a simultaneous eigenket of $\hat{H}$ and $\tau(a)$. It is an $\hat{H}$ eigenket is obvious because $|n\rangle$ is an energy eigenket with eigenvalue E_0, independent of n. Now,

$$\begin{aligned}\tau(a)|\theta\rangle &= \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle = \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}|n\rangle \\ &= e^{-i\theta}|\theta\rangle\end{aligned}$$

Thus, $|\theta\rangle$ is also an eigenket of the translation operator $\tau(a)$.
If we take a look at a more realistic situation, i.e., Figure 1(a) where the barrier between two adjacent lattice sites is not infinitely high. We can construct a localised ket $|n\rangle$ with properties as before $\tau(a)|n\rangle = |n+1\rangle$. However, this time we expect some leakage to be possible into neighboring lattice sites as a consequence of quantum-mechanical tunneling. In other words, the wave function has a tail extending to sites other than the n^{th} site. The diagonal elements of $\hat{H}$ in the $\{|n\rangle\}$ basis are all equal because of translation invariance; i.e.,

$$\langle n|\hat{H}|n\rangle = E_0$$

independent of n like before. However, like in the previous case here, the Hamiltonian $\hat{H}$ is not completely diagonal in the $\{|n\rangle\}$ basis as a consequence of leakage. Now, if we consider the barrier to be high (but not infinity), we assume that the wave function only leaks to its immediate neighbors, i.e.,

$$\langle n'|\hat{H}|n\rangle \neq 0 \qquad only\ \ if \qquad n' = n\ \ or\ \ n' = n \pm 1$$

This assumption is known as the *Tight-Binding Approximation* in solid-state physics. Now let us define

$$\langle n \pm 1|H|n\rangle = -\Delta$$

Thus our Hamiltonian is of the form,

$$H = \begin{bmatrix} E_0 & -\Delta & 0 & \dots & \\ -\Delta & E_0 & -\Delta & 0 & \dots \\ 0 & -\Delta & E_0 & -\Delta & \\ 0 & 0 & \ddots & \ddots & \ddots \end{bmatrix}$$

We see that Δ is again independent of n because of the translation invariance of the Hamiltonian such that $|n\rangle$ and $|n'\rangle$ are orthogonal to each other when $n \neq n'$. Thus we get

$$H|E_0, n\rangle = E_0|E_0, n\rangle - \Delta|E_0, n+1\rangle - \Delta|E_0, n-1\rangle$$

We see that $|n\rangle$, is no longer an energy eigenket.
Now let us again consider a linear combination as we did above,

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta} |E_0, n\rangle$$

which is an eigenket of translation operator $\tau(a)$ as we have shown above. Let us check if it's also an energy eigenket

$$\begin{aligned}
\hat{H}|\theta\rangle &= \sum_{n=-\infty}^{\infty} e^{in\theta} \hat{H} |E_0; n\rangle \\
&= \sum_{n=-\infty}^{\infty} e^{in\theta} [E_0 |E_0; n\rangle - \Delta |E_0; n+1\rangle - \Delta |E_0; n-1\rangle] \\
&= E_0 |\theta\rangle - \Delta e^{i\theta} |\theta\rangle - \Delta e^{-i\theta} |\theta\rangle \\
&= E_0 |\theta\rangle - \Delta (e^{i\theta} + e^{-i\theta}) |\theta\rangle \\
&= (E_0 - 2\Delta cos(\theta)) |\theta\rangle
\end{aligned} \tag{1}$$

We see that in this situation, the energy eigenvalues depend on the continuous real parameter θ. Also, the degeneracy is lifted as Δ becomes finite, and we have a continuous distribution of energy eigenvalues between $Eo - 2\Delta$ and $Eo + 2\Delta$.

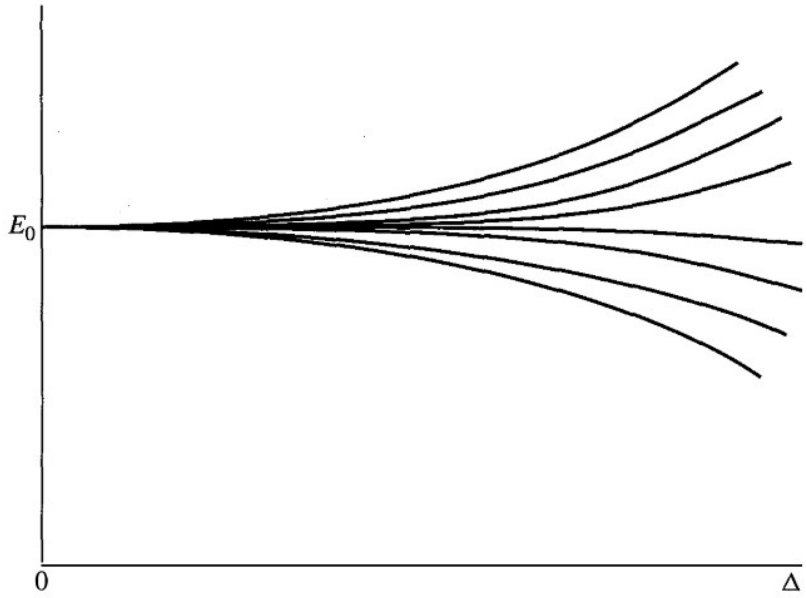


Figure 2: Energy levels forming a continuous energy band as Δ is increased from zero.

Let us now see the physical meaning of the parameter θ by studying the wavefunction $\langle x'|\theta\rangle$.

For the wave function of the lattice-translated state $\tau(a)\,|\theta\rangle$, we obtain

$$\begin{aligned}\langle x'|\,\tau(a)\,|\theta\rangle &= (\tau(a)^\dagger\,|x'\rangle)^\dagger\,|\theta\rangle \\ &= (|x'-a\rangle)^\dagger\,|\theta\rangle \\ &= \langle x'-a|\theta\rangle\end{aligned} \tag{2}$$

Now let us operate $\tau(a)$ on $|\theta\rangle$. Thus,

$$\begin{aligned}\langle x'|\,\tau(a)\,|\theta\rangle &= \langle x'|\,e^{-i\theta}\,|\theta\rangle \\ &= e^{-i\theta}\,\langle x'|\theta\rangle\end{aligned} \tag{3}$$

So,

$$\langle x'-a|\theta\rangle = e^{-i\theta}\,\langle x'|\theta\rangle$$

To solve this equation we setup

$$\langle x'|\theta\rangle = e^{ikx'}\,u_k(x')$$

with $\theta = ka$, where $u_k(x')$ is a periodic function with period a. thus the above equation becomes,

$$e^{ik(x'-a)}u_k(x'-a) = e^{ikx'}\,u_k(x')e^{-ika}$$

Thus we get the important condition known as *Bloch's Theorem*. The wave function of $|\theta\rangle$, which is an eigenket of $\tau(a)$, can be written as a plane wave $e^{ikx'}$ times a periodic function with periodicity a.

For further information you can look in the book Modern Quantum Mechanics by Sakurai [3]

3 Non-Relativistic Electrons

Dynamics of these systems is given by schrodinger equation, for our case we'll restrict ourselves to just time independent 1-D case. Time independent 1-D Schrodinger equation is given by,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{4}$$

For convenience we'll take $\hbar = 2m = 1$. We can now discretize the above equation, where variables are defined as below.

$$\begin{aligned} x &\in [a,b] \\ h &= \frac{b-a}{N+1} \\ x_n &= a + nh \\ n &\in \{0,1,2,\ldots,N+1\} \\ \psi_n &= \psi(x_n) \\ V_n &= V(x_n)\end{aligned}$$

here x_n gives the lattice points.

$$\psi_{n+1} + \psi_{n-1} = \left(2 - Eh^2 + V_n h^2\right)\psi_n \tag{5}$$

Periodic Potentials

For the case of periodic potentials with a period L,

$$V(x+L) = V(x)$$

We know from the *Bloch's Theorem* that,

$$\psi(x+L) = \exp(ikL)\psi(x) \tag{6}$$

Kronig-Penny Model

We want to get the band structure of the 1D lattice with atoms sitting at each lattice point (separated by L). In Kronig-Penny model we have infinite sequence of Dirac-Delta potential separated by L, making our potential periodic. We will model our problem (1D lattice) based on this simplified model.

Transfer Matrix Method

Before going into the detail computation of the *Transfer Matrix*, let's take a step back to properly define the problem. We have a periodic potential which repeats after L. To discretize this potential we'll use the similar method as we use to define the charge distribution of discrete charge distribution. As we know that the potential repeats after L, from *Bloch's Theorem* we know $\psi(x+L)$ if we know $\psi(x)$. Therefore the *Schrodinger's equation* becomes,

$$-\frac{d^2}{dx^2}\psi(x) + \left(\sum_n \lambda_n \delta(x-nh)\right)\psi(x) = E\psi(x) \tag{7}$$

here λ_n represents the strength of the potential at the x_n.

We can now use the *Poincare map* technique to get,

$$\psi_{n+1} + \psi_{n-1} = \left(2\cos\left(h\sqrt{E}\right) + \lambda_n \frac{\sin\left(h\sqrt{E}\right)}{\sqrt{E}}\right)\psi_n \tag{8}$$

we can simplify the expression by taking $h \to 0$[1].

$$\psi_{n+1} + \psi_{n-1} = \left(2 - Eh^2 + \lambda_n h\right)\psi_n \tag{9}$$

Note that if we substitute $\lambda_n = hV_n$ in [9] we exactly get [5], which means that the strength of the Dirac-delta potential is dependent on the value of the potential at that point. We can write the above recurrence relation in the following matrix form,

$$\begin{pmatrix}\psi_{n-1}\\ \psi_n\end{pmatrix} = \begin{bmatrix}2+h\lambda_n - h^2E & -1\\ 1 & 0\end{bmatrix}\begin{pmatrix}\psi_n\\ \psi_{n+1}\end{pmatrix} = P_n\begin{pmatrix}\psi_n\\ \psi_{n+1}\end{pmatrix} \tag{10}$$

$$\begin{pmatrix}\psi_{n-1}\\ \psi_n\end{pmatrix} = P_1P_2\ldots P_{N+1}\begin{pmatrix}\psi_{N-1}\\ \psi_N\end{pmatrix} \tag{11}$$

[1] Which essentially means that the lattice point for the solution is very close.

$$\begin{pmatrix}\psi_0\\ \psi_1\end{pmatrix} = T_{N+1}\begin{pmatrix}\psi_{N-1}\\ \psi_N\end{pmatrix} = T_{N+1}\exp(ikL)\begin{pmatrix}\psi_0\\ \psi_1\end{pmatrix} \tag{12}$$

Here T_{N+1} is the transfer matrix which takes the solution from the $N+1$ back to the 1. We can massage the above equations to get the following recurrence relation between T_N, T_{N+1} and T_{N-1},

$$(\mathbb{1} - T_{N+1}\exp\{iL\})\begin{pmatrix}\psi_0\\ \psi_1\end{pmatrix} = 0 \tag{13}$$

Now as the above column vector is non trivial this means that the determinant of the matrix must be zero, which gives us the following relation.

$$\cos kL = \frac{1}{2}Tr(T_{N+1}) \tag{14}$$

we can see that the following relation is true,

$$T_{N+1} = T_N P_{N+1} \tag{15}$$

when comparing the matrix elements we get the following recursion relation,

$$\begin{aligned} T^{11}_{N+1} &= (2 + h\lambda_{N+1} - h^2E)T^{11}_N - T^{11}_{N-1} \\ T^{22}_{N+1} &= (2 + h\lambda_N - h^2E)T^{22}_N - T^{22}_{N-1} \end{aligned} \tag{16}$$

as we have taken very small step we can assume that $\lambda_{N+1} \approx \lambda_N$, which gives us the following relation between the trace of the matrices.

$$Tr(T_{N+1}(E)) = \left(2 - h\lambda_{N+1} - h^2E\right)Tr(T_N(E)) - Tr(T_{N-1}(E)) \tag{17}$$

we also see that the following relation is true, where k is the momentum.

$$\cos(kL) = \frac{1}{2}Tr(T_{N+1}) \tag{18}$$

Here $Tr(T_N)$ represents trace of T_N. We also see that,

$$\begin{aligned} Tr(T_0) &= 2 \\ Tr(T_1) &= 2 + h\lambda_{N+1} - h^2E \end{aligned} \tag{19}$$

using the above relation, [17] and [18] we can estimate the band-structure of a non-relativistic electron in a 1D lattice.

4 Relativistic Electrons

Klein-Gordon Equation

Here we will go through the derivation of Klein-Gordon equation, which attempts to generalize the Schrodinger equation in the relativistic limits. we know from special relativity that

$$E^2 = m^2c^4 + p^2c^2 \tag{20}$$

by using the correspondence principle $p \to -i\hbar\nabla$,Hamiltonian operator can be written as

$$H^2 = m^2c^4 - c^2\hbar^2\nabla^2 \tag{21}$$

so our known Schrodinger equation,

$$i\hbar\frac{\partial\psi(t,x)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(t,x) \tag{22}$$

here we can square the operators on both sides and get this,

$$-\hbar^2\frac{\partial^2}{\partial t^2} = (m^2c^4 - c^2\hbar^2\nabla^2) \tag{23}$$

we can rearrange this and write in the following way

$$(\Box + \frac{m^2c^2}{\hbar^2})\psi = 0 \tag{24}$$

where $\Box = \frac{\partial^2}{c\partial t^2} - \nabla^2$ is the e d'Alembert operator. we can find the probability density from the above equation and it is given as

$$\rho = \frac{i\hbar}{2mc^2}(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\phi^*}{\partial t}) \tag{25}$$

this quantity can be negative, which is a major problem in Klein Gordon Equation.

Dirac Equation

The negative probability of the Klein-Gordon Equation was related to the fact that the Klein-Gordon equation is second order in time, Dirac decided to find a relativistic wave equation that was first order in time. so we write the Schrodinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{26}$$

but with some Hamiltonian to be determined.
Dirac reasoned that since his equation was first order in the time derivative and since relativity is supposed to treat space and time on an equal footing, it should also be first order in the spatial derivatives.
He guessed the Hamiltonian should be in the form

$$H = c\alpha.p + mc^2\beta \tag{27}$$

Here $\alpha = (\alpha_1, \alpha_2, \alpha_2)$ is a 3-component vector and $\mathbf{p} = -i\hbar\nabla$.
so the Dirac equation for a free particle can be written as

$$i\hbar\frac{\partial\psi}{\partial t} = -i\hbar c\sum_{k=1}^{3}\alpha_k\frac{\partial\psi}{\partial x_k} + mc^2\beta\psi \tag{28}$$

here $\psi = \begin{pmatrix} \psi_1 \\ \psi 2 \\ . \\ . \\ \psi_N \end{pmatrix}$ is a multi-component object called spinor and $\alpha_i' s$ and β are N X N matrices.$\alpha_i' s$ and β are hermitian since Dirac Hamiltonian is hermitian
the solution to the Dirac equation is also a solution to the Klein-Gordon Equation so applying $i\hbar\frac{\partial}{\partial t}$ with the above equation we get

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2} = H^2\psi = -\hbar^2c^2\sum_{kl}\alpha_k\alpha_l\frac{\partial^2\psi}{\partial x_k\partial x_l} - i\hbar mc^3\sum_{k=1}^{3}(\alpha_k\beta+\beta\alpha_k)\frac{\partial\psi}{\partial x_k} + m^2c^4\beta^2\psi \tag{29}$$

for the above equation to agree with the Klein-Gordon equation the following equation needs to be satisfied,

$$\frac{1}{2}(\alpha_k\alpha_l + \alpha_l\alpha_k) = \delta_{kl}, \quad \alpha_k\beta + \beta\alpha_k = 0, \quad \beta^2 = 1 \tag{30}$$

These constitute the Dirac algebra, the set of algebraic relations which the Dirac matrices α_k and β must satisfy

Finding the Dirac Matrices

from the Dirac algebra, we can easily show that $\alpha_k^2 = 1$ and $\beta^2 = 1$. this implies that the possible eigenvalues are ± 1. we also get

$$tr(\beta\alpha_k\beta) + tr(\alpha_k) = 0 \tag{31}$$

but by cycling the order of matrices we can write,

$$tr\beta\alpha_k\beta) = tr(\beta^2\alpha_k) = tr(\alpha_k) \tag{32}$$

which means $tr(\alpha_k) = 0$. in a similar way $tr(\beta) = 0$. buy since the eigenvalues are ± 1 N have to be even.
the simplest possibility is N=2. but if we do the calculation we can show that for N=2 there is no solution of the Dirac algebra. but for N=4 solution exists and one of the possible solutions is,

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{33}$$

where the 4 X 4 matrices are partitioned into four 2 X 2 matrices, which are represented in terms of Pauli matrices and the 2 X 2 identity matrix(indicated by 1) . for more information you can look into the following lecture notes [1]

Relativistic electrons in periodic potentials

one dimensional Dirac equation for an electron of mass=1/2 in a periodic potential V(x) of period L.in units $\hbar = c = 1$,is given below

$$-i\alpha\frac{d}{dx} + \frac{\beta}{2} + v(x) = E_R\psi(x) \tag{34}$$

,here $\psi(x)$ is the two component wavefunction, α and β are 2x2 traceless,Hermitian matrices and E_R is the relativistic energy of the electron.set $\alpha = \sigma_z$ and $\beta = \sigma_x, \sigma's$ being the Pauli matrices and $E = E_R - \frac{1}{2}$ and denoting by ϕ and χ the upper and lower components of the wave function, respectively, we obtain

$$[i\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\frac{d}{dx} + \frac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + v(x)]\begin{pmatrix}\phi(x)\\ \chi(x)\end{pmatrix} \tag{35}$$

$$\chi(x) = 2(i\frac{d}{dx} - v(x) + E + \frac{1}{2})\phi(x) \tag{36}$$

$$\phi(x) = 2(-i\frac{d}{dx} - v(x) + E + \frac{1}{2})\chi(x) \tag{37}$$

putting χ in this equation we get

$$[\frac{d^2}{dx^2} + V(x)^2 - (2E+1)V(x)\phi(x) + E(E+1)]\phi = 0 \tag{38}$$

, we will work with smooth potential and almost flat potential so we can neglect the term $\frac{dV}{dx}$. now we will break the length L into discrete length of length h where h is small. after discretizing the above equation we get

$$\phi_{n+1} + \phi_{n-1} = [2 - h^2(V_n + E(E+1) - (2E+1)V_n]\phi_n \tag{39}$$

by periodicity of potential we get $V_{n+N+1} = V_n$, and by Bloch theorem we get

$$\phi_{n+N+1} = exp(ikL)\phi_n \tag{40}$$

now we consider the Dirac equation for a periodic array of δ-function potentials

$$[-i\sigma_z\frac{d}{dx} + \sigma_x + \sum_n \delta(x - nh)]\psi(x) = (E + \frac{1}{2})\psi(x). \tag{41}$$

by Poincare map technique we get this

$$\begin{aligned}\phi_{n+1} &+ \exp(i\lambda_n - i\lambda_{n-1})\phi_{n-1}\\ &= \Big[2\cos\lambda_n \cos\Big(\sqrt{E(E+1)}h\Big)\\ &\quad + \frac{(2E+1)\sin\lambda_n \sin\Big(\sqrt{E(E+1)}h\Big)}{\sqrt{E(E+1)}}\Big]\phi_n\end{aligned} \tag{42}$$

in the limit $h \to 0$ and for smooth potential $\lambda_n, \lambda_{n-1} << 1$, so we have

$$\phi_{n-1} + \phi_{n+1} = [2 - (\lambda_n^2 + E(E+1)h^2 - (2E+1)\lambda_n h]\phi_n \tag{43}$$

by making the approximation that $\lambda_n \approx \lambda_{n-1} \approx \lambda_{n+1}$ we can write the above equation in matrix form in the following way

$$\begin{pmatrix}\phi_{n-1}\\ \phi_n\end{pmatrix} = \begin{pmatrix}2 - (E(E+1)h^2 + \lambda_n^2 - (2E+1)\lambda_n h) & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\phi_n\\ \phi_{n+1}\end{pmatrix} \tag{44}$$

for ease of writing we call $P_n = \begin{pmatrix} 2-(E(E+1)h^2+\lambda_n^2-(2E+1)\lambda_n h) & -1 \\ 1 & 0 \end{pmatrix}$, then we can write this in the following wave

$$\begin{pmatrix} \phi_{n-1} \\ \phi_n \end{pmatrix} = P_n \begin{pmatrix} \phi_n \\ \phi_{n+1} \end{pmatrix} \tag{45}$$

$$\begin{pmatrix} \phi_0 \\ \phi_1 \end{pmatrix} = P_1 P_2 ... P_{N+1} \begin{pmatrix} \phi_{N+1} \\ \phi_N \end{pmatrix} \tag{46}$$

we define $T_{N+1} = P_1 P_2 ... P_{N+1}$, and by *Bloch's Theorem* we get

$$\begin{pmatrix} \phi_0 \\ \phi_1 \end{pmatrix} = T_{N+1} exp(ikL) \begin{pmatrix} \phi_0 \\ \phi_1 \end{pmatrix} \tag{47}$$

for non-trivial solution we have

$$\begin{aligned} det(I - T_{N+1} exp(ikL)) = 0 \\ cos(kL) = \frac{1}{2} Tr(T_{N+1}) = F_{N+1}(E) \\ T_{N+1} = T_N P_{N+1} \end{aligned} \tag{48}$$

say $\alpha = 2-(E(E+1)h^2+\lambda_n^2-(2E+1)\lambda_n h)$, and we will assume $\lambda_{n+1} \approx \lambda_n \approx \lambda_{n-1}$

$$\begin{pmatrix} T_{N+1}^{11} & T_{N+1}^{12} \\ T_{N+1}^{21} & T_{N+1}^{22} \end{pmatrix} = \begin{pmatrix} T_N^{11} & T_N^{12} \\ T_N^{21} & T_N^{22} \end{pmatrix} \begin{pmatrix} \alpha & -1 \\ 1 & 0 \end{pmatrix} \tag{49}$$

$$\begin{pmatrix} T_{N+1}^{11} & T_{N+1}^{12} \\ T_{N+1}^{21} & T_{N+1}^{22} \end{pmatrix} = \begin{pmatrix} T_N^{11}\alpha + T_N^{12} & -T_N^{11} \\ T_N\alpha + T_N^{22} & -T_N^{21} \end{pmatrix} \tag{50}$$

compare the element of both the matrix we get

$$\begin{aligned} T_{N+1}^{11} = T_N^{11}\alpha + T_N^{12} \\ T_{N+1}^{12} = -T_N^{11} \\ T_{N+1}^{21} = T_N\alpha + T_N^{22} \\ T_{N+1}^{22} = -T_N^{21} \end{aligned} \tag{51}$$

by rearranging the above equations we get

$$\begin{aligned} T_{N+1}^{11} = \alpha T_N^{11} - T_N^{11} \\ T_{N+1}^{22} = \alpha T_N^{22} - T_{N-1}^{22} \end{aligned} \tag{52}$$

we define $F_N(E) = \frac{1}{2} Tr(T_N)$ and we know that $T_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $T_1 = P_1$ so we get

$$F_{N+1}(E) = \frac{1}{2}(T_{N+1}^{11} + T_{N+1}^2 2) = \alpha F_N(E) - F_{N-1}(E) \tag{53}$$

where $F_0(E) = \frac{1}{2} Tr(T_0) = 1$ and $F_1(E) = \frac{1}{2} Tr(T_1) = 1 - \frac{1}{2}(E(E+1)h^2 + \lambda_1^2 - (2E+1)\lambda_1 h)$
we have used this result to find the band structure by writing code in python. the result is shown below in the numerical analysis section .

5 Numerical Results

We've solved the equations that we have got above to get the 1D band structure for the following potential, with $N = 1000000$.

$$\begin{aligned} V(x) &= V_0 \cos(2x) \\ V_0 &= 0.2 \\ m &= 0.5 \end{aligned} \tag{54}$$

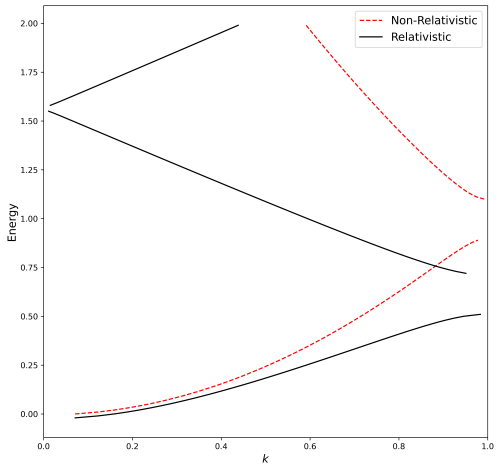
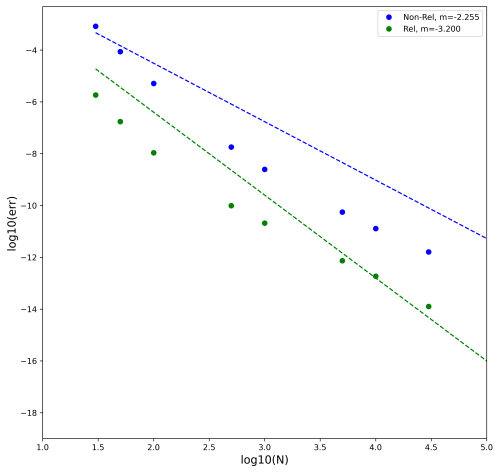


Table 1: Band limit for a non-relativistic particle of mass=0.5 in the potential $V(x) = 2cos(2x)$ compared with the exact value of energy(from the analytical solution of Mathieu potential

	N=200	N=20000	Exact Value
Upper Band	3.859	3.909	3.917
	1.990	1.860	1.859
Lower Band	-0.119	-0.12	-0.110
	-0.459	-0.449	-0.455

We can observe from the graph that relativity causes the shrinkage of the spectrum.

We've also numerically verified the claim made in [2] that the Poincare map approach and the discretization approach match as we make the step size small.



6 Conclusion

In this paper, we have demonstrated that the dynamics of both non-relativistic and relativistic particles in one-dimensional potentials are equivalent to the dynamics of particles in an array of δ- function potentials with different weight factors. In the case of a general periodic potential we have found that the dispersion relation is the same as that of a generalized kronig-penny model. This equivalence also shows why the Kronig penny model can explain the behaviour of electron in one-dimensional lattice.

The transfer matrix method allows us to obtain a very simple recursive method to compute $E(k)$,this reduces the computation time and storage, so this process can be used to find the band structure for any general smooth potential easily on any programming platform.

References

[1] Robert Littlejohn. *Klein-Gordon and Dirac Equation.* Physics 221AB, Quantum Mechanics, University of California, Berkeley, Fall 2019 and Spring 2020.

[2] B Mendez, F Dominguez-Adame, and E Macia. A transfer matrix method for the determination of one-dimensional band structures. *Journal of Physics A: Mathematical and General*, 26(1):171–177, January 1993.

[3] J.J Sakurai and J. Napolitano. *Modern Quantum Mechanics 2nd edition(2011):Jim Smith.*