

Representation of Energy Bands in a 1D Periodic Potential

Iñigo Urutiaga* and Luis Martínez†
Enginyeria Física, UPC

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The quantum mechanical equations that determine the electronic band structure of a perfectly periodic material can be approximately solved by truncation of the Fourier series of the interaction potential. For didactic purpose, a user friendly interface has been developed, designed to represent the bands arising from an adjustable spatially periodic potential in one dimension. In this work, we describe the use of the interface and apply the program to the particular case of an optical lattice.

I. INTRODUCTION

The crystalline structure of a solid can be thought of as being a periodic arrangement of atoms in space, which can be modeled in a first approximation as an infinite periodic lattice. In terms of the interactions between atoms in the solid structure, the lattice is described by a periodic potential which is determined by the properties of the material.

In this setting, the quantum mechanical theory predicts a discrete set of allowed energy states for the electrons inside the solid. In particular, the Bloch Theorem (see ch. 8 in [1]) shows that each state of the electron is determined by two quantum numbers n and k (also by the spin number, which is ignored). The allowed energy states for a fixed value of n define the energy bands, which are found to be continuous on the number k and describe a curve in the k -Energy plane. We think of k as a continuous quantity, despite taking discrete values which are close for a large number of atoms. For most potentials, the curves tend to be separated by gaps in the Energy coordinate, so many values of the energy are forbidden.

Curiously enough, energy bands are not only a theoretical phenomenon arising from the consideration of an infinite, perfectly periodic arrangement of atoms, but appear also in the band structure of real materials. The fact that solids admit energy bands has a profound impact on our understanding of the transport properties of materials, leading to the classification of conducting and insulating materials, and the development of important disciplines, such as physical electronics. Then, knowing the allowed energies for a solid and the energy gaps between them becomes crucial in material science.

Thus, it is interesting to be able to compute the energy bands for a particular potential. Although not physically exact, the infinite periodic approximation is sufficiently good so as to provide some insight into the shape of the bands in real solids. Remarkably enough, the electronic bands in a one dimensional system can be numerically obtained by solving an approximate eigenvalue equation,

which we discuss in detail in the next section below. Modeling the one dimensional case is much easier than doing it for higher dimensions, since it only allows one type of periodicity, while higher dimensions allow plenty of possible periodic lattices.

With the purpose of improving the intuition of Physics students and helping them to understand what an electronic band is and how it appears in crystalline structures, a user friendly interface has been developed in Matlab. The interface can be used as a complementary tool to the solid state physics course, allowing the student to try different potentials and motivating the study of the general theory.

II. THEORETICAL FOUNDATIONS

Consider the one electron Hamiltonian in 1D

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \quad (1)$$

corresponding to a periodic potential U such that $U(x) = U(x+a)$ for a fixed spatial parameter a defining a Bravais lattice (see ch. 4 in [1]).

Bloch's Theorem shows that the eigenstates of the hamiltonian can be chosen to have the form of a modulated plane wave

$$\psi_{nk}(x) = e^{ikx} u_{nk}(x), \quad u_{nk}(x) = u_{nk}(x+a) \quad (2)$$

where the amplitude has the periodicity of the lattice.

Since the potential is periodic, we may expand it in a Fourier series

$$U(x) = \sum_G U_G e^{-iGx} \quad (3)$$

with G a set of points in the reciprocal lattice ($G = n \frac{2\pi}{a}$ for integer n). The coefficients are easily found by numerical integration. Writing an arbitrary eigenfunction in the form

$$\psi(x) = \sum_k C_k e^{ikx} \quad (4)$$

where the k satisfy the Born-von Karman boundary condition (see ch. 8 in [1]), substituting in the Schrödinger

* inigo.urutiaga.erneta@gmail.com

† luis.martinez.zorooa@estudiant.upc.edu

equation and renaming terms, we obtain

$$\sum_G \frac{\hbar^2}{2m} C_{k-G} (k-G)^2 e^{i(k-G)x} + \quad (5)$$

$$+ \sum_G \sum_{G'} U_{G-G'} C_{k-G} e^{i(k-G)x} = E \sum_G C_{k-G} e^{i(k-G)x},$$

whence it follows that

$$\left(\frac{\hbar^2}{2m} (k-G)^2 - E \right) C_{k-G} + \sum_{G'} U_{G'-G} C_{k-G'} = 0. \quad (6)$$

For each k , we define $\lambda_k = \frac{\hbar^2}{2m} k^2$ and set our units of energy and length to $\frac{\hbar^2}{2ma^2}$ and a , respectively.

Considering only a finite number of Fourier coefficients in the expansion of ψ , we obtain for each k a linear system which can be diagonalized. In this approximation, the eigenvalues of this system, labeled by the number n , correspond to the allowed energies for a fixed k . By varying k in the first Brillouin zone ($-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$), we can plot the electronic bands in this representation. As an example of the linear system to solve, we show the equations assuming $C_{k+mG} = 0$ for $|m| > 1$:

$$\begin{pmatrix} \lambda_{k+G} - E & U_{-G} & U_{-2G} \\ U_G & \lambda_k - E & U_{-G} \\ U_{2G} & U_G & \lambda_{k-G} - E \end{pmatrix} \begin{pmatrix} C_{k+G} \\ C_k \\ C_{k-G} \end{pmatrix} = 0 \quad (7)$$

In the final implementation of the program, a 51×51 linear system is solved for a total number of 2000 values of k in the first Brillouin zone. The number $N = 51$ corresponds to the number of coefficients considered in the truncation of the Fourier series of the potential. For larger values of N , the computed bands are found to converge to the same curve, as seen in figures 1 and 2, so the truncation is a good approximation to the real solution. Likewise, considering more values of k increases the resolution of the curves in the plot. For 2000 points the continuity of the bands is clearly seen, so no more resolution is needed.

III. DESCRIPTION OF THE INTERFACE

The program is divided into two files with extension .fig and .m, respectively. The former contains the graphical design of the interface, which consists of several blocks with associated callback functions. These functions determine the purpose of each block, and are programmed in the latter file, which contains the Matlab code where the main program and algorithms are implemented, namely: energy band computation, external/user-introduced variable acquiring, and data visualization.

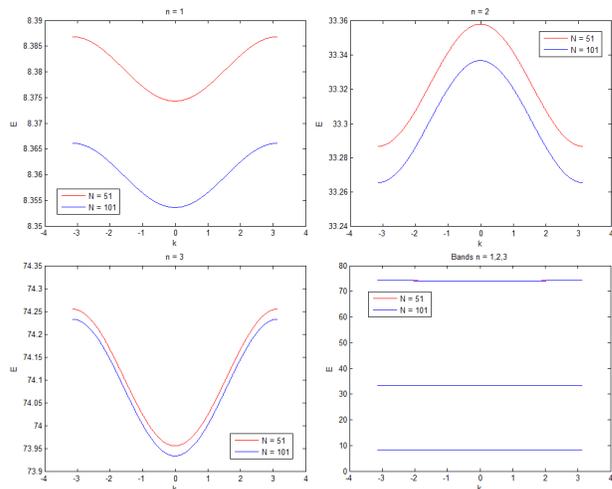


Figure 1. Lower bands for $N = 51$ and $N = 101$ in a sawtooth potential of depth $V_0 = 200$. The shape of the bands is independent of the approximation, while a small difference in height can be observed. Observe that this difference is negligible when compared with the band separation, so that the same bands are obtained in practice.

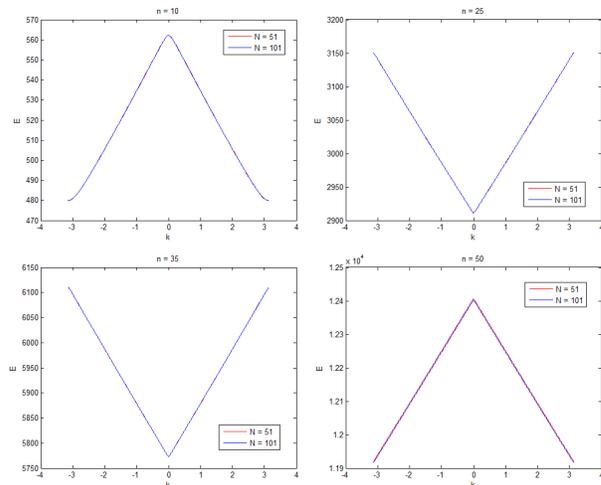


Figure 2. Intermediate and high bands for $N = 51$ and $N = 101$ in a sawtooth potential of depth $V_0 = 200$. The curves between the least and the most energetic bands converge to the same graph, while notable differences begin to appear for the band with n close to N .

When executing the program, a window as the one in figure 3 is opened. In this window, several blocks and buttons can be seen, which we now describe.

First of all, the two big boxes on the left and right are for the plots of the periodic potential and the corresponding energy bands, respectively.

On the upper half of the window, near the center, a pop-up menu can be found. This menu allows the user to choose a particular potential among the following:

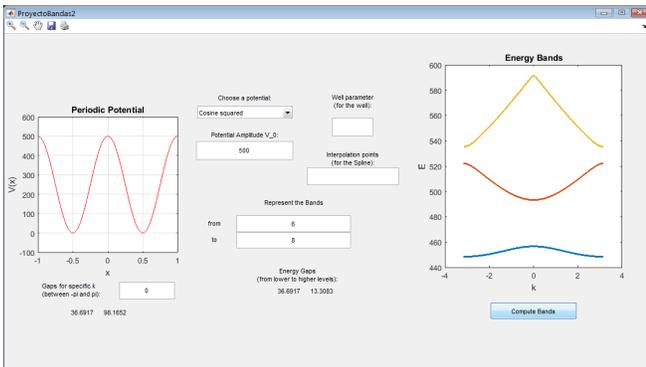


Figure 3. Interface menu.

a. *Cosine potential.* The most simple potential, it has only one Fourier coefficient. The frequency of the potential coincides with that of the spatial lattice, so it repeats after a distance a ($= 1$ as our unit of length).

b. *Cosine squared potential.* This potential is found in optical lattices, and we study it extensively later. In order for the potential to have a periodicity a , the cosine must be taken with half the frequency as before. Thus, it is similar to the former case, since

$$V_0 \cos^2\left(\frac{x}{2a}\right) = \frac{V_0}{2} + \frac{V_0}{2} \cos\left(\frac{x}{a}\right). \quad (8)$$

c. *Potential well.* One of the most famous potentials in theoretical mechanics, the potential is defined as

$$V(x) = \begin{cases} V_0 & |x| \leq a/2h \\ 0 & |x| > a/2h \end{cases} \quad (9)$$

for $-a/2 \leq x \leq a/2$, and periodically extended. The *well parameter* box allows the user to change the width h of the potential.

d. *Sawtooth potential.* An asymmetric potential in the shape of a sawtooth signal, defined in each lattice unit by the formula:

$$V(x) = \frac{V_0}{2} + \frac{V_0}{a}x. \quad (10)$$

The potential is 0 at $x = -a/2$ and V_0 at $x = a/2$.

e. *Coulomb potential.* The periodic Coulomb potential accounts for the presence of atomic nuclei in the lattice. Due to its long-range character, the effect of every atom must be taken into account, which is computationally unrealizable. As a consequence, only the effect of a finite number of adjacent atoms has been considered. Moreover, being a singular potential, its Fourier coefficients cannot be effectively computed and approximate integrals must be used. The resulting bands depend strongly on the number of atoms considered and the integral approximation, so no realistic results can be found. Despite this, the approximate bands have been included, so that the user gains some qualitative insight into how the bands look like. A rigorous treatment of the subject can be found in the study of Wigner crystals (see [6]).

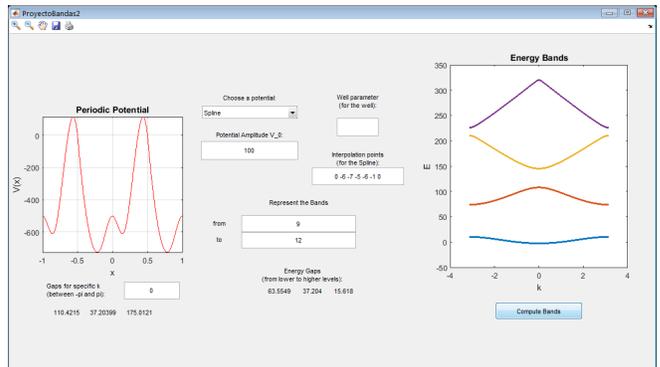


Figure 4. Energy bands in a spline potential. The points in the graph are chosen to approximate any function.

f. *Adjustable potential (Spline potential).* The most interesting potential, due to its generality. The program offers the possibility to create an arbitrary periodic potential by choosing different y coordinates for its graph. These coordinates define evenly spaced points that are interpolated with a third degree spline, which is periodically extended to obtain the wanted potential. To insert the desired coordinates, the user may simply write the associated $V(x)$ of the predefined x points in the form of an array inside the box with the label *Interpolating points*. See figure 4 for an example of a spline function.

Once the potential is chosen, several parameters can be adjusted. In order to modify these, the smaller white blocks are used. The user may change the values inside the blocks by clicking the corresponding box and writing the desired parameters with the keyboard. After pressing enter, the plot of the new potential is updated.

Finally, when every parameter has been fixed, the user may press the button on the lower-right side to compute the energy bands. After a few seconds, the graphs of the bands are shown on the right canvas. The user can also decide which bands to plot by changing the numbers in the boxes *from* and *to*. As the names suggest, the bands with quantum numbers n between the values in *from* and *to* are represented. This allows the user to observe the differences in curvature between the different allowed energy bands arising from the potential.

Furthermore, the energy gaps are also computed, in two ways. In the center of the interface, the minimum separation between each consecutive gap is shown in ascending order, while on the bottom-left side a particular value of k can be chosen, so that the energy gaps for that value are calculated. The first number gives the user an idea of the order of magnitude of the gaps between consecutive bands, while the second value accounts for a specific gap difference.

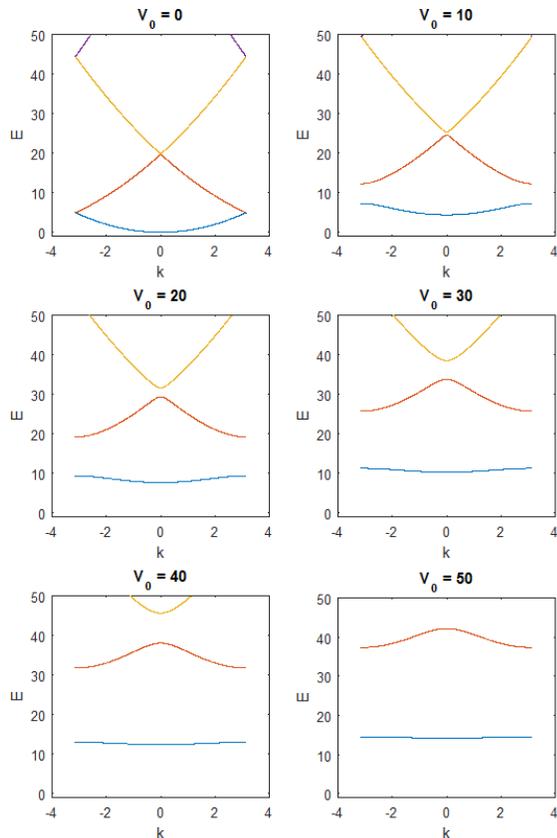


Figure 5. Representation of the electronic bands for the cosine squared potential, for different potential depths.

IV. EXAMPLE: 1D OPTICAL LATTICE

We show an example of application of the program to optical lattices, which are nowadays of clear practical

interest in modern quantum physics (see [2] or [4]).

In this system, two counter-propagating laser waves of the same frequency interfere, leading to a standing wave and a spatially periodic potential for atoms of the form

$$V(x) = V_0 \cos^2 \left(\frac{2\pi}{\lambda} x \right), \quad (11)$$

where λ is the wavelength of the lasers. This potential is used by experimental physicists to confine atoms inside the potential minima, forming a periodic array of particles and thus creating an artificial solid.

As stated earlier, our program considers a cosine squared potential of the form as in eq. (8), so taking $a = \lambda/2$ as our unit of length, we can model a 1D optical lattice and we may compute the energy bands of the particular system.

In figure 5, we show the electronic bands corresponding to the quantum numbers $n = 1, 2, 3$ for different potential depths, as obtained with the program. Observe that the energy gaps between bands become larger for a larger potential depth. In solid state physics, a high energy gap between a filled band and an empty band corresponds to an insulator. Thus, we see that controlling the potential depth of an optical lattice allows the physicist to control the transport properties of the new material. We see also that for a sufficiently high potential depth the variation of the lower bands is small compared with the energy gaps. This means that the low energy bands tend to be flatter when compared with the band separation.

For a general potential, the behaviour of the electronic bands is similar. The bands with the lowest energy tend to be flat with respect to the energy gaps, while the high energy bands are close to the parabolas corresponding to free electrons. For energies of the order of the potential depth, interesting curvatures can be found, as the ones that we find in a solid.

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