Hofstadter's Butterfly in Hexagonal Lattice

The project

The project is done as part of Ulpanat De Shalit 2006, a two weeks summer programme for undergraduate physics students in the Weizmann institute.

The project was created along with Chen Tradulsky under the guidance of Ariel Amir and Dr. Yuval Oreg. Our purpose was to investigate the effect of static magnetic field on the energy structure of square and hexagonal lattices. The energy band graph which is created is known as Hofstadter's bufferfly. The code for this project was written in MATLAB and can be found here. The project was presented using a PowerPoint presentation that can be found here.

Lattice energy structure and Hofstadter's Butterfly

In order to determine the energy structure of a lattice one has to first create it's Hamiltonian and then diagonalize it in order to extarct the eigenvalues. In this project we've built the Hamlitonian from hypothetical base function. In order to build and diagonalize the Hamiltonian in a simple manner we used the Tigh Binding approximation, according to which we needed only to consider the interaction between each base function to it closest neighbours. We marked the non-zero terms of the Hamiltonian as :

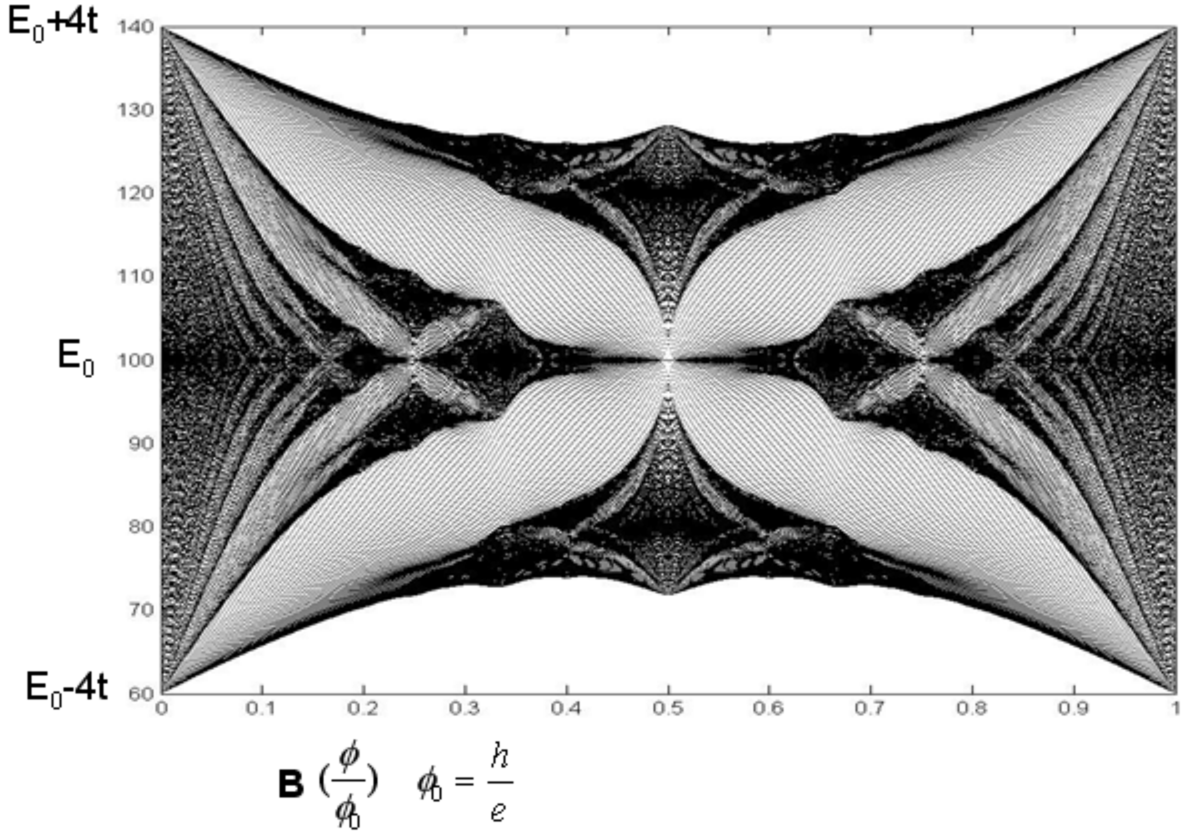
$$\langle\psi(r)|\psi(r)\rangle = E_0 \qquad \langle\psi(r)|\psi(r\pm a\hat{x})\rangle = t \qquad \langle\psi(r)|\psi(r\pm a\hat{y})\rangle = t$$

From here on the diagonalization is very simple, especially when it's done numerically using MATLAB. The result is a single energy band. However, when we add magnetic field the terms of interaction are added a phase which is an integral of the potential vector :

$$\langle\psi(r)|\psi(r\pm a\hat{x})\rangle = t\exp(\pm\frac{i}{\hbar}\int\vec{A}d\hat{x}) \qquad \langle\psi(r)|\psi(r\pm a\hat{y})\rangle = t\exp(\pm\frac{i}{\hbar}\int\vec{A}d\hat{y})$$

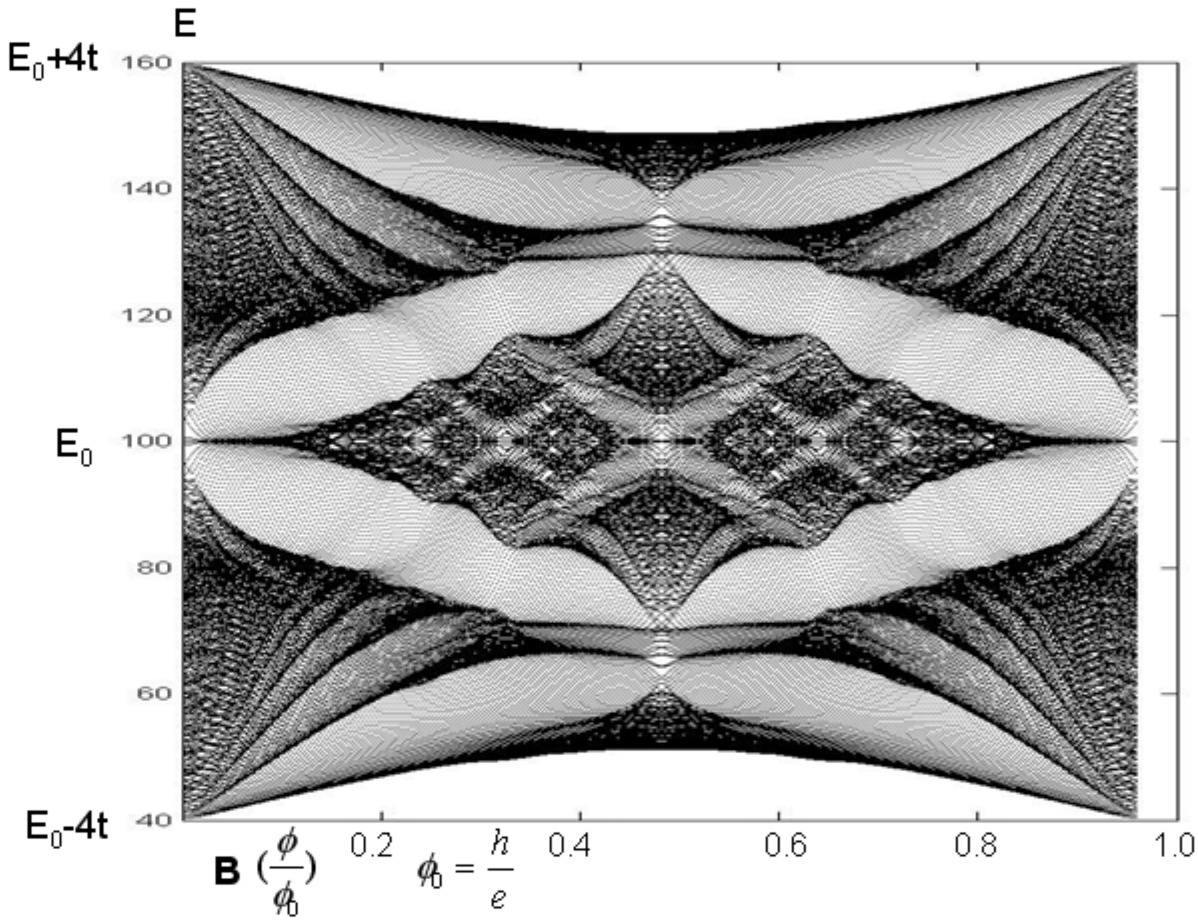
When we diagonlize this we get a complex energy band which changes in a chaotic manner with the magnetic field. The result is the graph called Hofstadter's butterfly. This pattern repeats itself when the magnetic flux through a unit cell reach the quantum flux unit.

Hofstadter's bufferfly in a square lattice :



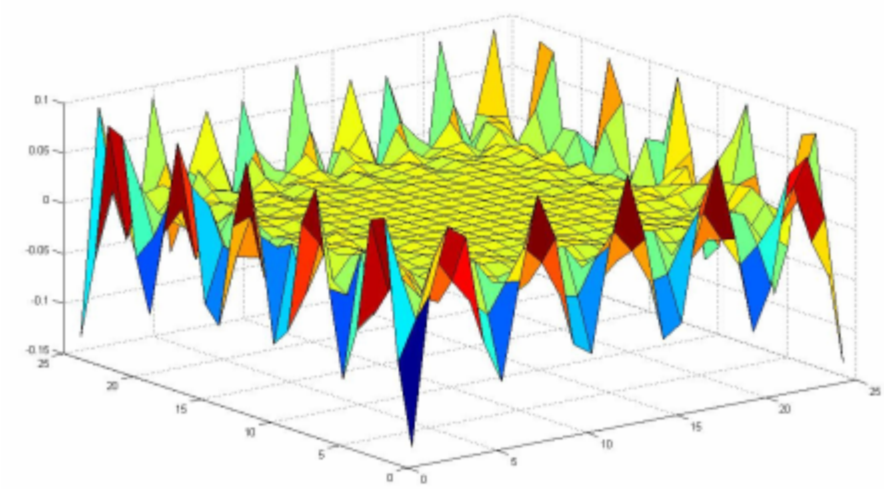
We have done the same thing in a two dimensional hexagonal lattice, though here the construction of the Hamiltonian is a bit more complicated.

Hofstadter's bufferfly in a hexagonal lattice :



Boundary Eigenstates

The gray areas are energies where there is a low density of states. Had we used a true infinite lattice these areas would have been completely empty. Therefore we expect the eigenfunction that exist there to be strongly effected by the finite boundry conditions as show in the following graph.



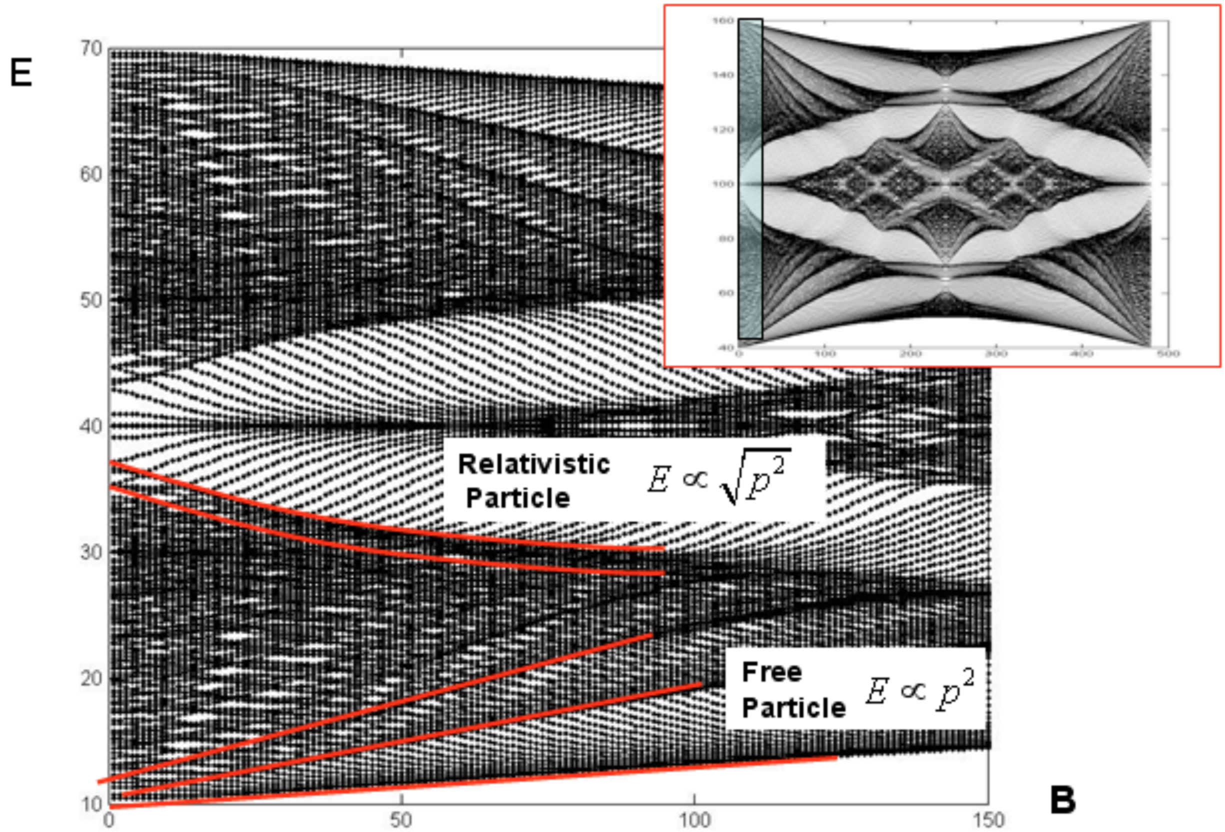
The following animation shows the evolution of an eigenstate along with the magnetic field - [eigenstate evolution animation].

Dispersion relations

The magnetic field required to see these affects is very high. However, many interesting effect can be seen when only considering low magnetic fields. In the hexagonal lattice on can clearly see stripes of high density of states. When calculating the dispersion relation for B=0 in the hexagonal lattice is can by analytically calculated as :

$$\varepsilon_{(k)} = E_0 - 2t\cos(2\pi k_y a) - 4t\cos(\pi k_x a\sqrt{3})\cos(\pi k_y a) + \sqrt{1+4\cos^2(\pi k_y a)+4\cos(\pi k_y a)\cos(\pi k_x a\sqrt{3}}$$

In the egde of the First Brillouin Zone this become similar to the dispersion of relativistic particle, and at it's center it becomes the dispersion relation of a free particle. The affect of low magnetic field on a free particle is known as Landau Levels that are discrete energy levels created as a result of the field. These level and similar ones created for the reletivistic particle can be seen in the following graph :


E
B
Relativistic Particle $E \propto \sqrt{p^2}$
Free Particle $E \propto p^2$
70
60
50
40
30
20
10
0
50
100
150