Square lattice in Magnetic Field

Student: Ido Friedler, Advisers: Eytan Grosfeld, Daniel Ariad

March 2018

Hofstadter's Law: It always takes longer than you expect, even when you take into account Hofstadter's Law.

1 Introduction

1.1 2-D Square lattice

The 2-D Square lattice Hamiltonian, assuming nearest neighbor tight-binding model

$$H = T_x + T_y + h.c. \tag{1}$$

where T_x, T_y are the translation operators,

$$T_x = -t \sum_{m,n} \psi^\dagger_{m+1,n} \psi_{m,n} \tag{2}$$

$$T_y = -t \sum_{m,n} \psi^\dagger_{m,n+1} \psi_{m,n} \tag{3}$$

Lets transform the hamiltonian to the momentum space:

$$\psi_{m,n} = \frac{1}{N} \sum_{k_x,k_y} e^{ik_x ma + ik_y na} C_{k_x,k_y} \tag{4}$$

where $N = L_x X L_y$
If so, the translation operator is:

$$\begin{aligned} T_x = &- t \sum_{m,n} \psi^\dagger_{m+1,n} \psi_{m,n} = -t \frac{1}{N^2} \sum_{m,n} \sum_{k_x,k_y} \sum_{\tilde{k_x},\tilde{k_y}} e^{-ik_x(m+1)a - ik_y na} e^{i\tilde{k_x} ma + i\tilde{k_y} na} C^\dagger_{k_x,k_y} C_{\tilde{k_x},\tilde{k_y}} = \\ &- t \frac{1}{N^2} \sum_{m,n} \sum_{k_x,k_y} \sum_{\tilde{k_x},\tilde{k_y}} e^{ima(\tilde{k_x} - k_x)} e^{ina(\tilde{k_y} - k_y)} e^{ia(\tilde{k_x})} C^\dagger_{k_x,k_y} C_{\tilde{k_x},\tilde{k_y}} = \\ &- t \frac{1}{N} \sum_{k_x,k_y} \sum_{\tilde{k_x},\tilde{k_y}} \delta_{k_x,\tilde{k_x}} \delta_{k_y,\tilde{k_y}} e^{iak_x} C^\dagger_{k_x,k_y} C_{\tilde{k_x},\tilde{k_y}} = -t \sum_{k_x,k_y} e^{iak_x} C^\dagger_{k_x,k_y} C_{k_x,k_y} \end{aligned} \tag{5}$$

asumming boundary conditions, $L_x a(\tilde{k} - k) = 2\pi p$, $L_y a(\tilde{k} - k) = 2\pi p, p \in N$, allowed us to get the Kronecker delta -

$$\sum_{m=1}^{L} e^{ima(\tilde{k} - k)} = \sum_{m=1}^{L} (e^{ia(\tilde{k} - k})^m = L \delta_{\tilde{k},k} \tag{6}$$

Now lets recall that we have the hermitian conjugate, so one can see -

$$\begin{aligned} &- t \sum_{m,n} (\psi^\dagger_{m+1,n} \psi_{m,n} + \psi^\dagger_{m,n} \psi_{m+1,n}) = \sum_{k_x,k_y} (e^{iak_x} + e^{-iak_x} C^\dagger_{k_x,k_y} C_{k_x,k_y} = \\ &- 2t \sum_{k_x,k_y} cos(k_x a) C^\dagger_{k_x,k_y} C_{k_x,k_y} \end{aligned} \tag{7}$$

having the same treatment to T_y yeilds

$$T_y = -2t \sum_{k_x,k_y} cos(k_y a) C^\dagger_{k_x,k_y} C_{k_x,k_y} \tag{8}$$

so finally we get:

$$H = -2t(\sum_{k_x,k_y} cos(k_x a) + cos(k_y a)) C^\dagger_{k_x,k_y} C_{k_x,k_y} \tag{9}$$

1.2 Magnetic field

Now we will add a perpendicular homogeneous magnetic field

$$\overrightarrow{B} = (0, 0, B) \tag{10}$$

We would like to express the magnetic field with $\overrightarrow{A}$, the vector potential, such that:

$$\overrightarrow{B} = \bigtriangledown X A \tag{11}$$

1.2.1 Peierls substitution

The Peierls substitution method is a widely employed approximation for describing tightly-bound electrons in the presence of a slowly varying magnetic vector potential.
In the presence of an external vector potential $\overrightarrow{A}$ the translation operators are simply -

$$T_x = -t \sum_{m,n} \psi^\dagger_{m+1,n} \psi_{m,n} e^{i\theta^x_{m,n}} \tag{12}$$

$$T_y = -t \sum_{m,n} \psi^\dagger_{m,n+1} \psi_{m,n} e^{i\theta^y_{m,n}} \tag{13}$$

and the peierls phase is -

$$\theta^x_{m,n} = \frac{e}{\hbar} \int_{ma}^{(m+1)a} A_{x,n} dx, \theta^y_{m,n} = \frac{e}{\hbar} \int_{na}^{(n+1)a} A_{y,m} dy \tag{14}$$

If so, the total phase gained due to one cell would be:

$$\phi_{m,n} = \theta^x_{m,n} + \theta^y_{m+1,n} - \theta^x_{m,n+1} - \theta^y_{m,n} \tag{15}$$

and, since the magnetic field is homogeneus $\phi_{m,n} \equiv \phi$, for any m,n

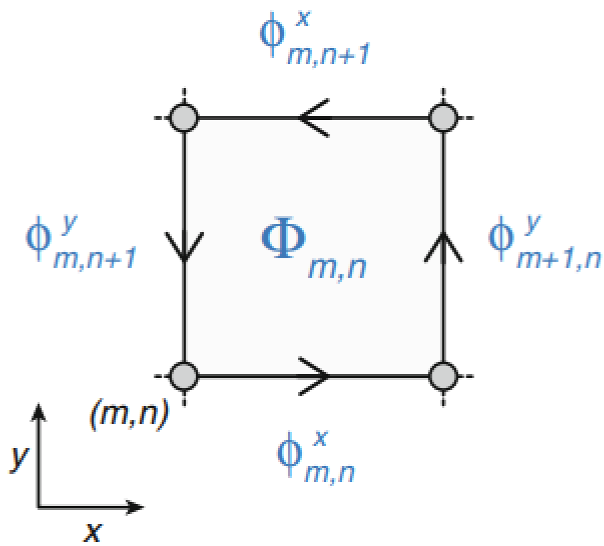


Figure 1: taken from [1]

1.2.2 Landau gauge

First lets define the magnetic flux quantum $\Phi_0 = \frac{h}{e}$
The Landau gauge is -

$$\overrightarrow{A} = B(0, x, 0) \tag{16}$$

in our case, x is discrete, and since we have periodic boundary conditions, and the phase is modulo 2π we get:

$$A = \frac{\Phi_0 p}{L}(0, m, 0), \quad p = 0..L - 1 \tag{17}$$

This gauge has an advantage that with this gauge the Hamiltonian commutes with y, as we will see later.
The total phase gained through one cell would be:

$$\phi = \theta^y_{m+1,n} - \theta^y_{m,n+1} = \frac{e}{\hbar}(\int_{na}^{(n+1)a} A_{m+1,y}dy - \int_{na}^{(n+1)a} A_{m,y}dy) = \frac{eap}{L\hbar} \tag{18}$$

taking $a = 1$, we get

$$\phi = \frac{2\pi p}{L}, \quad p = 0..L - 1 \tag{19}$$

Note: since $a = 1$ the phase is dimensionless.

The magnetic flux of one cell would be:

$$\Phi = \frac{\Phi_0 p}{L} \tag{20}$$

The total flux from the system would be the sum of L^2 cells:

$$\Phi_{tot} = L^2\Phi = \Phi_0 Lp, \quad p = 0..L-1 \tag{21}$$

and by changing the magnetic field:

$$\Delta\Phi_{tot} = \Phi_0 L \tag{22}$$

Plugging in the magnetic field in the Hamiltonian leads us to Harper equation [2]. With the chosen gauge the derivation of T_x stays the same as Eq. 5-7, but now with the magnetic field the T_y expression changes.

$$\begin{aligned} &= -t\sum_{m,n} e^{i\frac{2\pi pm}{L}}\Psi^\dagger_{m,n+1}\Psi_{m,n} = \\ &= -t\frac{1}{N^2}\sum_{m,n} e^{i\frac{2\pi pm}{L}}\sum_{k_x,k_y}\sum_{\tilde{k_x},\tilde{k_y}} e^{-ik_x ma - ik_y(n+1)a}e^{i\tilde{k_x}ma + i\tilde{k_y}na}C^\dagger_{k_x,k_y}C_{\tilde{k_x},\tilde{k_y}} \end{aligned} \tag{23}$$

and now we get the condition:

$$\sum_{m=1}^{L} e^{\frac{i2\pi mp}{L}}e^{m(\tilde{k_x}-k)} = \sum_{m=1}^{L} e^{i(\tilde{k_x}-k_x+\frac{2\pi mp}{L})^m} = L\delta_{\tilde{k_x},k_x-\frac{2\pi p}{L}} \tag{24}$$

and similarly for the Hermitian conjugate we would get: $L\delta_{\tilde{k_x},k_x+\frac{2\pi p}{L}}$
Lets define $\phi = \frac{p}{L}$ some rational number, so now our Hamiltonian would be:

$$H = \sum_{k_x,k_y} -2tcos(k_x)C^\dagger_{k_x,k_y}C_{k_x,k_y} - te^{ik_y}C^\dagger_{k_x-2\pi\phi,k_y}C_{k_x,k_y} - te^{-ik_y}C^\dagger_{k_x+2\pi\phi,k_y}C_{k_x,k_y} \tag{25}$$

This Hamiltonian is diagonal in k_y but mix k_x with $k_x \pm 2\pi\Phi$, so now lets define $k_x = \tilde{k_x} + 2\pi\phi n$ and change the borders of k_x from the range $-\pi < k_x < \pi$ to $-\frac{\pi}{L} < \tilde{k_x} < \frac{\pi}{L}$ so the Hamiltonian can be rewritten:

$$H = \sum_{\tilde{k_x},k_y} H_{\tilde{k_x},k_y} \tag{26}$$

$$\begin{aligned} H_{\tilde{k_x},k_y} = &\sum_{n=0}^{L-1}(-2tcos(k_x+2\pi\phi n)C^\dagger_{k_x+2\pi\phi n,k_y}C_{k_x+2\pi\phi n,k_y} - te^{-ik_y}C^\dagger_{k_x+2\pi\phi(n+1),k_y}C_{k_x+2\pi n,k_y} \\ &- te^{ik_y}C^\dagger_{k_x+2\pi\phi(n-1),k_y}C_{k_x+2\pi\phi n,k_y} \end{aligned} \tag{27}$$

This Hamiltonian does not couple different $\tilde{k_x}$ or k_y , so we can just study a particular block with fixed $\tilde{k}_x$ and k_y So using the $H_{\tilde{k_x},k_y}$, so the Schrodinger equation

$$H_{\tilde{k_x},k_y}|\Psi>=E_{\tilde{k_x},k_y}|\Psi> \tag{28}$$

Assume that the state can be expanded as

$$|\Psi>=\sum_{m=0}^{L-1} a_m C^{\dagger}_{\tilde{k_x}+2\pi\Phi m,k_y}|0> \tag{29}$$

Then we obtain

$$\begin{aligned}&\sum_{m=0}^{L-1}(-2tcos(\tilde{k_x}+2\pi\Phi m)C^{\dagger}_{\tilde{k_x}+2\pi\Phi m,k_y}a_m - te^{-ik_y}C^{\dagger}_{\tilde{k_x}+2\pi\phi(m+1),k_y}a_m \\ &- te^{ik_y}C^{\dagger}_{\tilde{k_x}+2\pi\phi(m-1),k_y}a_m = E_{\tilde{k_x},k_y}\sum_{m=0}^{L-1}C^{\dagger}_{\tilde{k_x}+2\pi\phi m,k_y}a_m\end{aligned} \tag{30}$$

and for the $n'th$ block we get:

$$-2tcos(\tilde{k_x}+2\pi\Phi n)a_n - t(e^{-ik_y}a_{n-1}+e^{ik_y}a_{n+1}) = E_{\tilde{k_x},k_y}a_n \tag{31}$$

1.2.3 Almost anti-symmetric gauge

For the almost anti-symmetric case, first we will define again the lattice size,

$$L_x = L_y + 1, L_y = L \tag{32}$$

Now we will define $\overrightarrow{A}$ -

$$A = \Phi_0 p(\frac{n}{L+1}, \frac{m}{L}, 0), \quad p = -..L(L+1)-1 \tag{33}$$

If so, the total phase gained through one cell would be

$$\begin{aligned}\phi =&\theta^x_{m,n} + \theta^y_{m+1,n} - \theta^x_{m,n+1} - \theta^y_{m,n} = \\ &= \frac{e}{\hbar}(\int_m^{(m+1)} A_{x,n}dx + \int_n^{(n+1)} A_{y,m+1}dy - \int_{(n+1)}^n A_{x,n+1}dx - \int_{(m+1)}^m A_{y,n}dx) = \\ &= \frac{e}{\hbar}(\frac{n\Phi_0 p}{L+1} + \frac{(m+1)\Phi_0 p}{L} - \frac{(n+1)\Phi_0 p}{L+1} - \frac{m\Phi_0 p}{L}) = \\ &= 2\pi p(\frac{n}{L+1} + \frac{m+1}{L} - \frac{n+1}{L+1} - \frac{m}{L+1}) = 2\pi p\frac{1}{L(L+1)}\end{aligned} \tag{34}$$

The magnetic flux of one cell would be:

$$\Phi = \frac{\Phi_0 p}{L(L+1)} \tag{35}$$

and the total flux would be:

$$\Phi_{tot} = \Phi_0 p \quad p = 0..L(L+1) - 1 \tag{36}$$

and by changing the magnetic field:

$$\Delta\Phi_{tot} = \Phi_0 \tag{37}$$

By comparing the Landau gauge and the almost anti-symmetric gauge one can notice that although the two systems have the same properties, and the maximal magnetic flux is the same order of L, $\Phi_{tot,max} \propto \Phi_0 L^2$, the almost anti-symmetric gauge allows us to examine the system with much higher resolution of the magnetic flux.

1.3 Hall effect

The classic Hall effect is a famous phenomenon by which a current flows perpendicularly to an applied voltage, or vice versa a voltage develops perpendicularly to a flowing current.
The Hall conductivity would be:

$$\sigma_H = \frac{n_e ec}{B} \tag{38}$$

although the classic phenomena does not have any quantum properties, we can notice that the Hall conductivity is independent by the size of the system, which might suggest us that the phenomena has special properties.
The quantum Hall effect is a quantum-mechanical version of the Hall effect, observed in two-dimensional electron systems subjected to low temperatures and strong magnetic fields, in which the Hall conductance σ_{xy} undergoes quantum Hall transitions to take on the quantized values:

$$\sigma_{xy} = \nu \frac{e^2}{h} \tag{39}$$

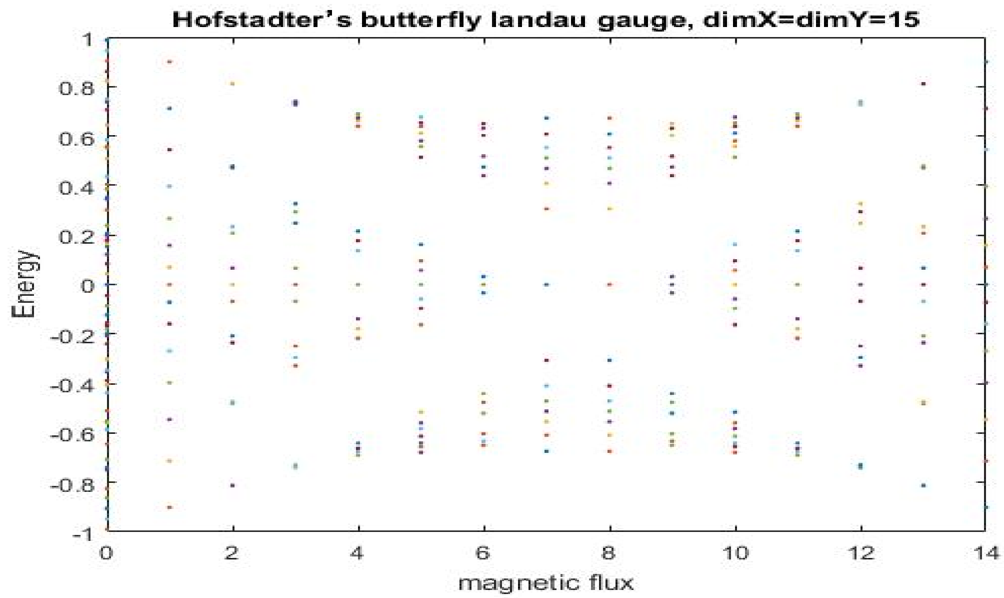
With magnetic field, we know that we have Landau degeneracy, and the electrons density depends on the magnetic field, so once we have strong magnetic field, the degeneracy is massive, and we would get that although we might change the magnetic field, the conductivity would not change.

2 Numerical results

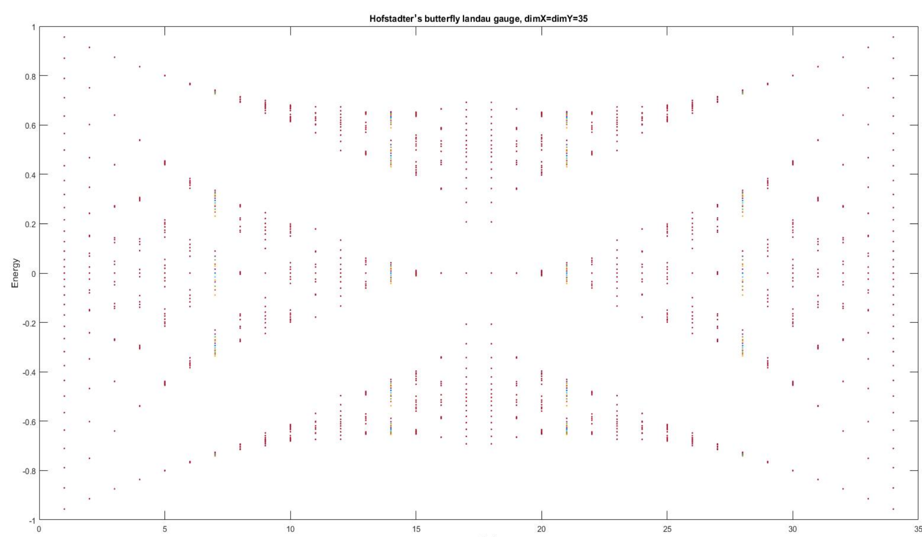
2.1 Hofstadter Butterfly

2.1.1 Landau gauge

Lets start with the Landau gauge as written in Eq. 17, with a lattice size $dimX = dimY = 15$

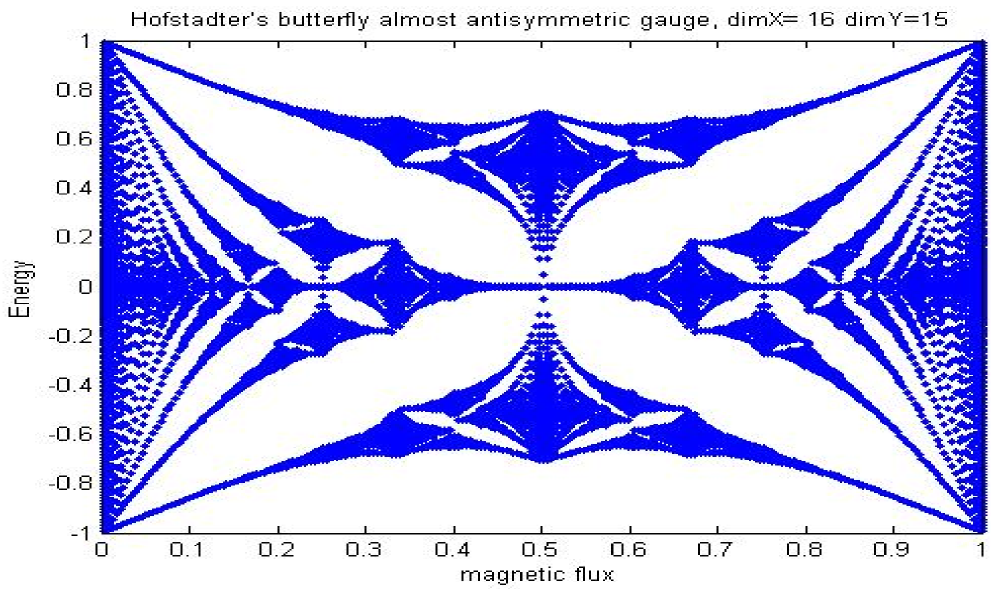


We can see the butterfly structure. To have a better look on the butterfly structure, lets take a bigger size of the lattice, with the same gauge $dimX = dimY = 35$



2.1.2 Almost antisymetric gauge

Now lets take a lattice with the size $dimX = 16, dimY = 15$



We can see that as we discussed before, the butterfly structure has a much better resolution altough the system dimensions are the same as the first figure in the Landau gauge

2.1.3 The Hofstadter Butterfly

Now that we have the Hofstadter Butterfly [3] we can discuss its significance. First we can notice that the spectrum has a fractal structure. We can recognize that we have big gaps in the structure, this will lead us to the Quantom Hall effect. In addition to that, we can see that in the low magnetic field and low energy regime we have a linear behavior of the energy, that will be discussed further more later.

2.2 Hall effect

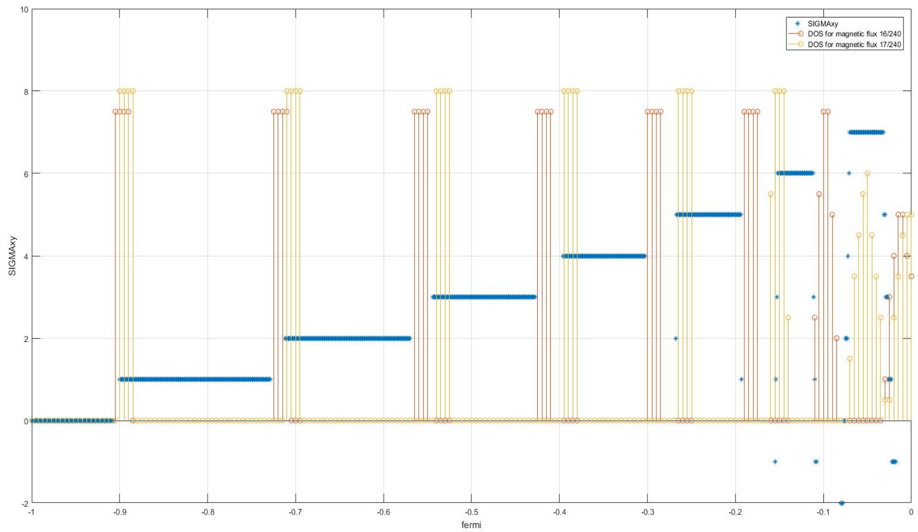
The Hall conductivity can be calculated using Streda formula [5]

$$\sigma_{xy} = -e\frac{\partial n}{\partial B}|_{\mu} \tag{40}$$

where n is the electron density.

$$\sigma_{xy} = -e\frac{\partial n}{\partial B}|_{\mu} = \frac{e^2}{h}\frac{N_{ef}(\phi + \Delta\phi) - N_{rf}(\phi)}{\Delta\phi} \tag{41}$$

where $N_{ef}(\phi)$ is the number of levels below the fermi energy with the total flux ϕ through the system.



The Hall conductivity depends on the spectrum at ϕ and the spectrum at $\phi + 1$ In this graph we can see the Hall conductivity as a function of Fermi energy, and the density of states for magnetic flux of 16/240 and 17/240 in red and yellow correspondly. We can see that the hall conductance values are pure integers multiplied by $\frac{e^2}{h}$. We can see that we have results the same as [4] .

2.3 Low energy and weak field

Lets examine the low energy and weak field case.
We start with the Hamiltonian from Eq. 9:

$$H = -2t \sum_{k_x, k_y} (cos(akx) + cos(aky))$$

Now lets recall Taylor expansion: $cos(x) \cong 1 - \frac{x^2}{2}$
By taking the low energy and low magnetic field limit,

$$H = H_0 + ta^2 k_x^2 + ta^2 k_y^2 \tag{42}$$

after adding magnetic field, using Landau gauge as shown in Eq. 17

$$H = H_0 + ta^2 k_x^2 + ta^2 (k_y - Bx)^2 \tag{43}$$

lets define: $ta^2 \equiv \frac{1}{2m}$, then we get:

$$H = H_0 + \frac{k_x^2}{2m} + \frac{(eB)^2}{2mc^2} (\frac{ck_y}{eB} - x)^2 \tag{44}$$

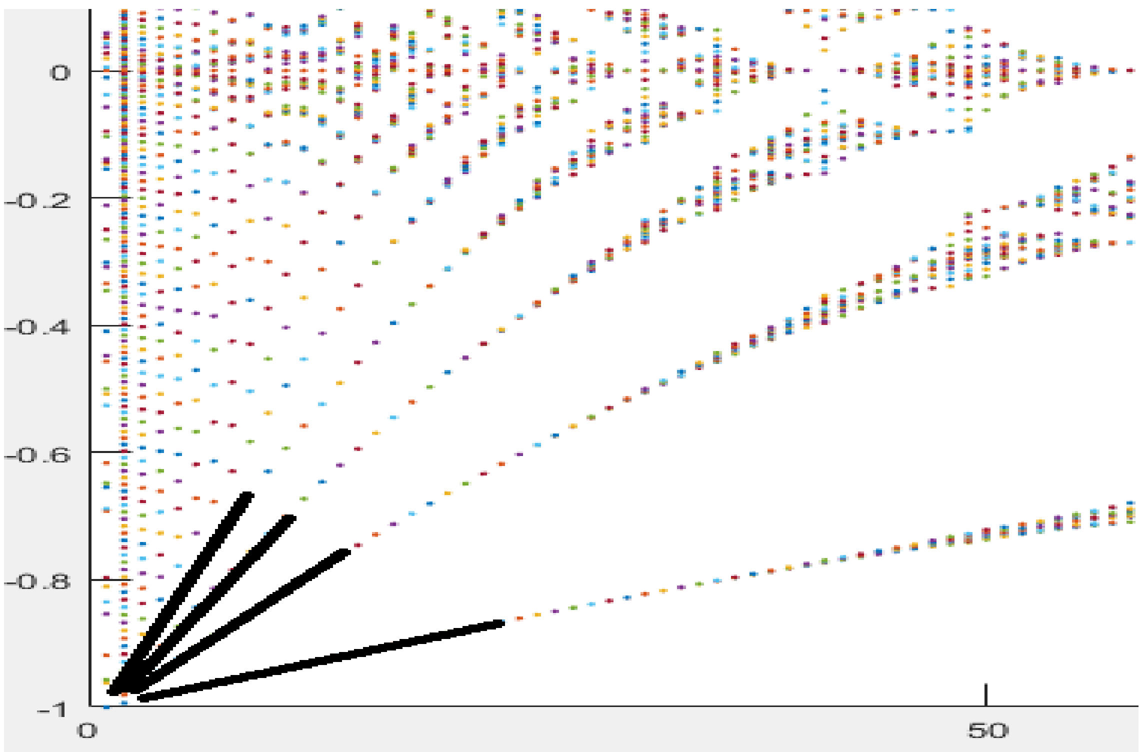
Now we can see that k_y commutes with the Hamiltonian, since there is no y operator in the Hamiltonian with the Landau gauge. Thus the operator k_y can be replaced by a number. The Hamiltonian can also be written more simply by noting that the cyclotron frequency is $\omega_b = qB/mc$, and removing H_0, giving

$$H = \frac{k_x^2}{2m} + \frac{\omega_b^2}{2m}(x - \frac{k_y}{m\omega_b})^2 \tag{45}$$

Now we can see that this is exactly like the quantum harmonic oscillator Hamiltonian, with a shifted coordinate space by $x_0 = \frac{k_y}{m\omega_b}$, thus the energies of the system are:

$$E_n = \hbar\omega_b(\frac{1}{2} + n) \tag{46}$$

which means that the energy is linearized by the magnetic field. By zooming in to the spectrum in the Hofstadter butterfly we can see that in the low energies and low magnetic field case, indeed we get linearized relation.



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