Numerical Norm Estimates For Certain Types of Harper Operators

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Introduction

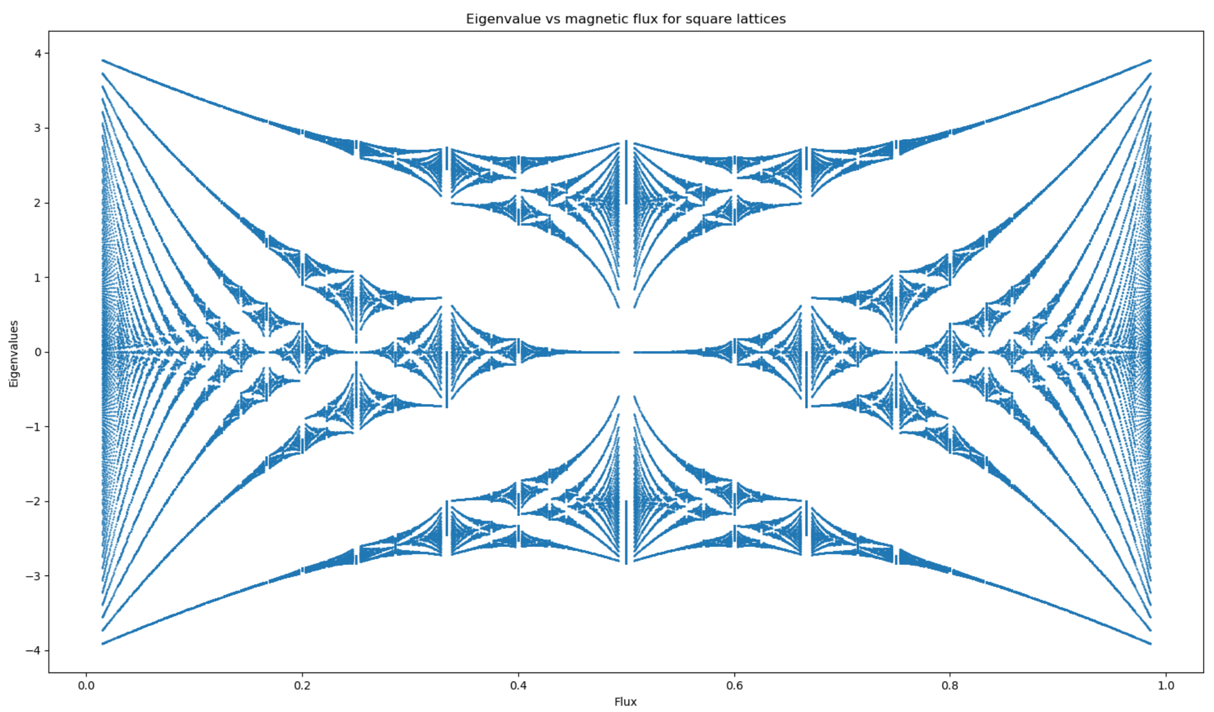
Goal:

The goal of this project is to generate models of the effects of magnetic fields on the energy states of electrons within multiple atomic lattices: square, triangular, and hexagonal.

Set Up:

The energy states of the electrons correspond to the eigenvalues of the Hamiltonian operator. The scope of our research mainly falls on the state of max energy, corresponding to the largest ab-solute value of the eigenvalues, i.e. the norm of the Hamiltonian at different values for magnetic flux $\alpha \in \mathbb{Q}$. This is important because the electrons with the highest energy states are the first to be stripped away when ionizing a molecule, so our results will show how easily a crystalline lattice can be ionized. We will use the Chambers formula to find the norm of the Hamiltonian, and plot the norm versus the magnetic flux applied to the lattice.

Mathematical Background



Hofstadter butterfly calculated using the Harper Operator for square lattices showing the eigenvalue vs magnetic flux (p/q for $q \leq 50$, (p, q) = 1).

Harper Operators

We define the unitary qxq matrices u and v, which satisfy the Weyl commutation relation $uv = e^{2\pi i p/q} vu$:

$$u = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ 1 & 0 & 0 & \dots & 0 \end{bmatrix} \qquad v = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & e^{1(2\pi i p/q)} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & e^{(q-1)(2\pi i p/q)} \end{bmatrix}$$

A theorem from Operator Algebras shows that the spectrum of the self-adjoint Hamiltonian H is given by:

$$\text{spec}(H) = \bigcup_{\theta_1, \theta_2 \in [0, 2\pi]} \text{spec}(M(\theta_1, \theta_2, \eta))$$

Harper Operators

The self-adjoint $q \times q$ matrices M are given by:

$$M_H(\theta_1, \theta_2) = e^{i\theta_1} u + e^{-i\theta_1} v + e^{i\theta_2} u^* + e^{-i\theta_2} v^*$$

in the case of a square lattice,

$$M_T(\theta_1, \theta_2, \eta) = M_H(\theta_1, \theta_2) + e^{-i\eta} e^{i(\theta_1+\theta_2)} uv + e^{i\eta} e^{(\theta_1+\theta_2)} v^* u^*$$

in the triangular lattice. and

$$M_G(\theta_1, \theta_2)^2 = M_T(\theta_1, \theta_2, 0) + 3I$$

in the case of the hexagonal lattice, which appears also in the analysis of the graphene.

Chambers Formula

The Chambers' formula allows us to find the norm of the Hamiltonian, and plot the norm versus the magnetic flux applied to the lattice. Chambers' formula represents the characteristic polynomial of $M_H(\theta_1, \theta_2)$ in the following forms for square and triangular lattices respectively:

$$\det\big(M_H(\theta_1, \theta_2) - xI\big) = p(x) + (-1)^{q+1} \cdot 2(\cos q\theta_1 + \cos q\theta_2)$$

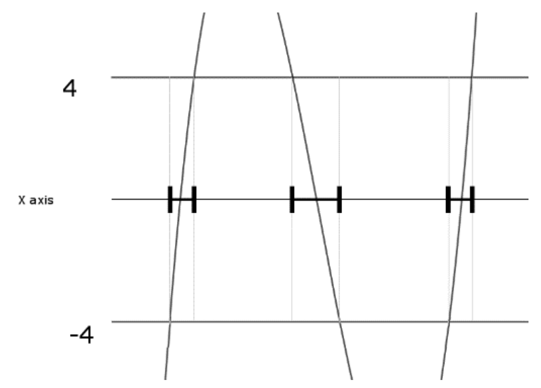
$$\det\big(M_H(\theta_1, \theta_2, \eta) - xI\big) = p(x) - 2\big(\cos q\theta_1 + \cos q\theta_2 + (-1)^{q+1} \cdot \cos[q(\theta_1 + \theta_2 - \eta)]\big)$$

where $p(x)$ is a polynomial of degree q.

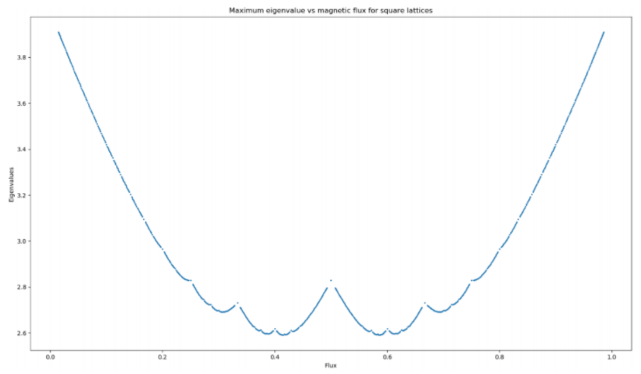
Results

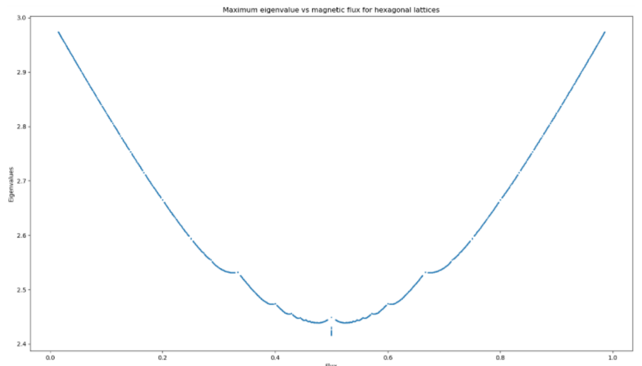
Generating the Bands for Each Lattice

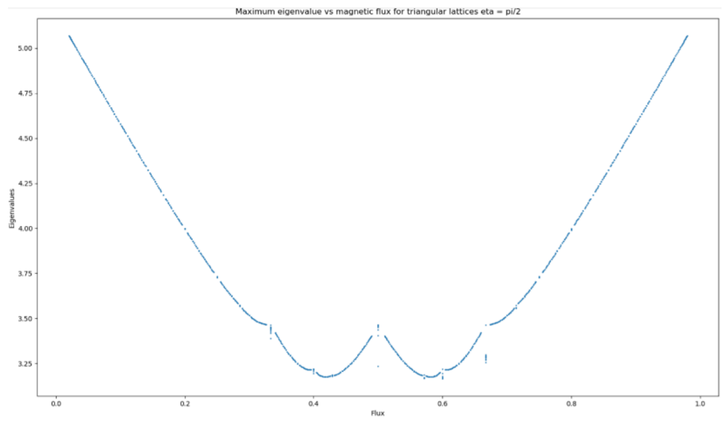
To retrieve the largest eigenvalue for multiple rational magnetic flux (p/q), we first calculated the values of θ_1 and θ_2 that would result the min and max values of the non-polynomial term in the Chambers formula. The eigenvalues of H are precisely the x's such that p(x) is between this min and max.



Definition. *Square lattice, Eigenvalues marked with brackets*







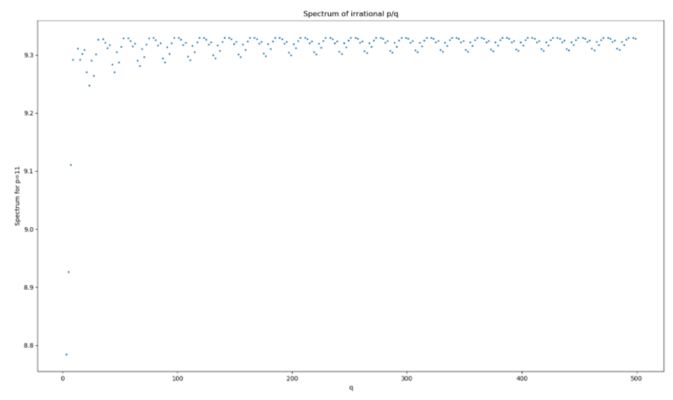
Maximum Eigenvalues of Square, Triangular, and Hexagonal Lattices for magnetic flux p/q ($q \leq 50$, (p, q) = 1, $\eta = \frac{\pi}{2}$).

Thouless Conjecture

The Thouless Conjecture states that:

$$q \cdot \lambda(spec(H_{p/q})) \xrightarrow[\gcd(p,q)=1]{q \to \infty} \frac{32 C_{cat}}{\pi} \approx 9.3299$$

Where C_{cat} is the Catalan constant, roughly 0.916.



Displays the Spectrum of irrational p/q

Future Directions

- Verify whether a Thouless-type conjecture is true for triangular and hexagonal lattices
- Verify whether the maximum eigenvalue of a square lattice is always greater than $2\sqrt{2}$ when $\frac{p}{q} \in \left[0, \frac{1}{4}\right] \cup \left[\frac{3}{4}, 1\right]$

References

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[2] F.P. Boca, A. Zaharescu, Norm estimates of almost Mathieu operators, J. Funct. Analysis 220 (2005), 76-96.

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[4] D.J. Thouless, Scaling for the discrete Mathieu equation, Comm. Math. Phys. 127 (1990), 187-193.

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