Numerical norm estimates for some classes of Harper type operators

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1 Introduction

The goal of this project is to generate models of the effects of magnetic fields on the energy states of electrons within atomic lattices. We are analyzing three different types of lattices: square, triangular, and hexagonal. One application of our research is on the properties of graphene, a carbon allotrope with a hexagonal lattice. Graphene is an extremely durable material with high thermal and electrical conductivity.

2 Harper Operators

The Hamiltonian operator is the energy operator for the system and can be approximated by a self-adjoint Harper- type operator. The eigenvalues of the Hamiltonian are the energy levels of the electrons. Thus we just need to find the spectrum of the Harper operator. Define U and V to be the following $q \times q$ unitary matrices

$$U = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ 1 & 0 & 0 & \dots & 0 \end{bmatrix} \qquad V = \begin{bmatrix} v_1 & 0 & 0 & \dots & 0 \\ 0 & v_2 & 0 & \dots & 0 \\ 0 & 0 & v_3 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & v_q \end{bmatrix}$$

where $v_n = e^{(n-1)*2i\pi(p/q)}$, n=1,2,...,q-1, and U^* and V^* are their adjoints. The matrices U and V satisfy the Weyl commutation relation $UV = e^{2\pi ip/q}VU$. A theorem from Operator Algebras shows that the spectrum of the self-adjoint Harper operator H is given by

$$\text{spec}(H) = \cup_{\theta_1,\theta_2\in[0,2\pi]}\text{spec}(M_H(\theta_1,\theta_2)),$$

where each M_H is a self-adjoint $q \times q$ matrix which is given by :
Square lattice: $M_H(\theta_1, \theta_2) = e^{i\theta_1}U + e^{-i\theta_1}U^* + e^{i\theta_2}V + e^{-i\theta_2}V^*$

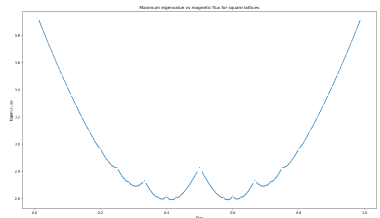
Triangular lattice: $M_T(\theta_1, \theta_2, \eta) = M_H(\theta_1, \theta_2) + e^{\theta_1+\theta_2-\eta}UV + e^{\theta_1+\theta_2+\eta}U^*V^*$

Therefore, the problem of finding the spectrum of H is reduced to finding the eigenvalues of each $M_H(\theta_1, \theta_2)$. We use the Chambers formula for the characteristic polynomial. In what follows, $f^H_{p,q}(x)$ is a polynomial of degree q, not depending on θ_1, θ_2.

Square lattice: $\det(M_H(\theta_1, \theta_2) - xI) = f^H_{p,q}(x) - (-1)^{q-1}2[\cos(q\theta_1) + \cos(q\theta_2)]$
Triangle lattice: $\det(M_T(\theta_1, \theta_2, \eta) - xI) = f^T_{p,q}(x) - 2[\cos(q\theta_1) + \cos(q\theta_2) + (-1)^{q+1}\cos(q(\theta_1 + \theta_2 - \eta))]$

3 Finding the largest eigenvalue

We find the maximum and minimum of the trigonometric term of the above characteristic polynomials. The eigenvalue with the greatest magnitude will be one of the roots of the cases where that term is minimized or maximized. The graph below plots flux against the maximum eigenvalue for M_H.

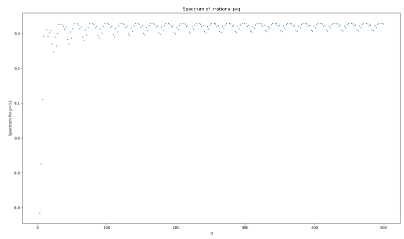


4 The Thouless Conjecture

A side project of our IGL research was numerically verifying the Thouless conjecture, which states that

$$\lim_{q\to\infty}(q * \lambda(\text{spec})(H_{p/q})) = \frac{32G}{\pi}$$

where $H_{p/q}$ is the energy operator for the flux p/q, λ is Lebesgue measure, and G is the Catalan constant, roughly 0.916. The image below shows the convergence to $\frac{32G}{\pi}$.



5 References

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