# Chern Numbers and Critical Exponents in Tight-Binding and Related Models

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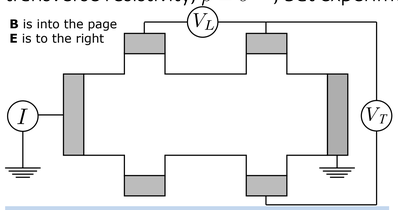
## Motivation

Conduction on microscopic scales behaves vastly differently than for larger sizes. A cornerstone the microscopic theory of solids is the Quantum Hall Effect, where with perpendicular electric and magnetic fields, the conductivity, $\sigma$, transforms from a continuous variable to a discrete variable $\sigma = c \cdot e^2/2\pi\hbar$, for integers $c$. These integers are known as the Chern numbers, and are determined from the electronic band structure. Depending on physical conditions, such as a change in electric or magnetic field, the Chern number for a system may change. This change is a phase transition, and like transitions between states of matter, the rate of transition may be described by a critical exponent, $\nu$.

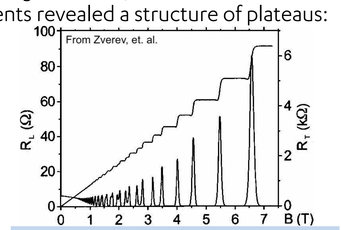
Here, we present a background on microscopic electronic behavior. Next, we develop a class of bound electron models. Finally, we find their Chern numbers and critical exponents by way of determining electronic band structures.

## Background

It was expected from the quantum theory that a Hall Experiment (a current in a two dimensional material with a perpendicular magnetic field), would exhibit a linear transverse resistivity, $\rho = \sigma^{-1}$, but experiments revealed a structure of plateaus:

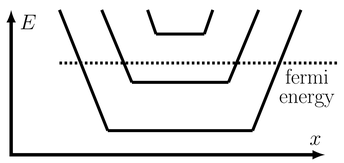



**Hall Bars are used to study electric properties of two dimensional materials in electric and magnetic fields.**

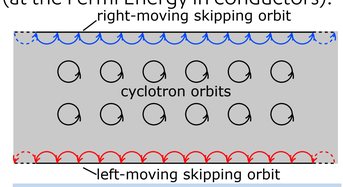



**Transverse resistivity plateaus at Landau Levels; longitudinal resistivity peaks at transitions.**

Nature strives to minimize energy, yet fermions such as electrons cannot "condense" to the ground state (because of the exclusion principle), so electrons build up to a highest occupied energy level known as the Fermi Energy. Electrons conduct at the lowest unoccupied energy level (at the Fermi Energy in conductors):



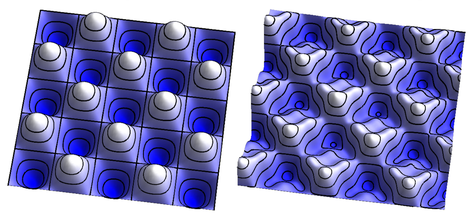

**The energy gap present in the bulk of a sample disappears near edges where "edge states" conduct left or right handed wrt the magnetic field.**




**An edge state conducting right adds one, and an edge state conducting left removes one from the Chern number.**

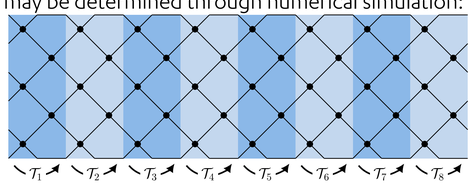
Around the center of each energy band, such as a Landau Level, in the presence of disorder, electrons may conduct. This region is known as the mobility edge:

**Electrons only conduct at the mobility edge: higher energy electrons loop on hilltops, lower energy electrons loop in valleys. Past a critical level of disorder, even mobility edge electrons can no longer move.**



Conductivity may be rephrased in terms of the distance an electron is localized to. Picturing the mobility edge of an energy band as a collection of contours and saddles, this "localization length" may be determined through numerical simulation:

**Strip models consider electronic systems that are much longer than they are wide. Localization is inversely related to transmission: $\xi \propto 1/\mathcal{T}$ with $\mathcal{T} \equiv \mathcal{T}_1\mathcal{T}_2 \ldots \mathcal{T}_N$**




## Methods

Quantum mechanics postulates that all information on the state of a system is contained by a vector $|\psi\rangle$, known as the wavefunction. Inner products extract the system information. We are interested with position in particular, so, for the system of four wells $m = 1, 2, 3, 4$, shown at right, $\langle m|\psi\rangle$ gives the probability amplitude that the particle is in the $m$-th well. Supposing that the particle is in the $m$-th well, we may move it right or left using a translation operator, $T_{\pm x}|m\rangle = |m \pm 1\rangle$, or let it be, $T_0|m\rangle = |m\rangle$. The translation operators are sums over outer products weighted by the transfer integrals $t$:

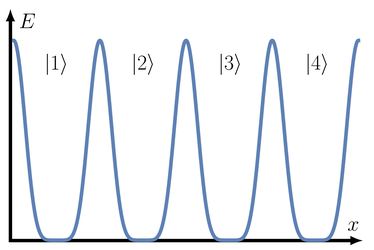
$$T_x = -\sum_m t_x|m+1\rangle\langle m|, \quad T_0 = -\sum_m t_0|m\rangle\langle m|, \quad T_{-x} = -\sum_m t_x|m\rangle\langle m+1|$$

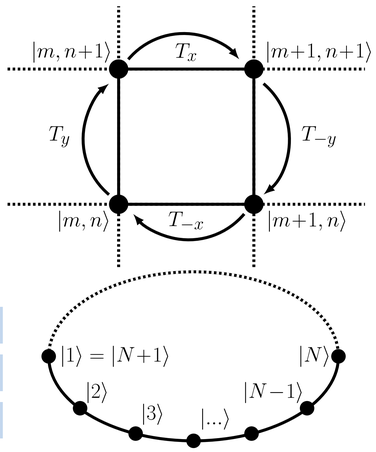
The Hamiltonian, a matrix of the possible configurations and motions, is the sum of the translation operators here, which is for a two-dimensional lattice:

$$H = T_0 + T_1 = T_0 + T_x + T_{-x} + T_y + T_{-y}$$

This Hamiltonian is a "tight-binding" Hamiltonian, which alludes to the separate wells, $m$, that the particle is "bound" to. The translation operators provide a formalism for conduction. Yet, in numerical simulations, only finite size systems may be studied, so boundary conditions must be specified. A simple and physically justified boundary condition is that of periodic boundaries.

With the Hamiltonian and its boundary conditions, the band geometries may be determined through matrix diagonalization. From this, the Chern numbers may be determined with some computation. Similarly, the localization length may be determined using the transfer matrix formalism and $QR$-factorization.




**Top: one-dimensional potential with four wells separated by barriers**

**Middle: translation operators can describe the motions of a particle**

**Bottom: periodic boundary conditions are illustrated with connection**

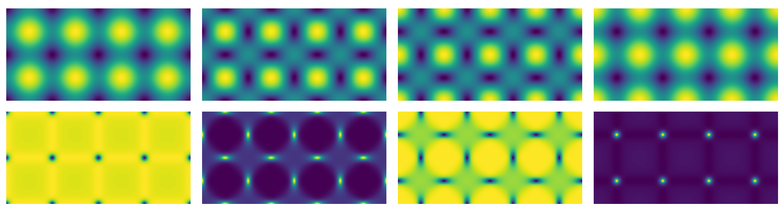
## Chern Numbers and Band Geometries

The Chern Number may be calculated as a momentum-space integral over the Brillouin zone over the Berry curvature. The Berry curvature, or field strength, may be calculated from the Berry connection $A(k)$. Where the Berry connection, is found from the wave functions $|n(k)\rangle$ of the $n$-th energy band. An efficient algorithm by Fukui *et. al.* was implemented.

$$A_i(k) = \left\langle n(k) \middle| \frac{\partial}{\partial k_i} \middle| n(k) \right\rangle; \qquad F(k) = \frac{\partial}{\partial k_1}A_2(k) - \frac{\partial}{\partial k_2}A_1(k); \qquad c_n = \frac{1}{2\pi i}\int_{BZ} d^2k\, F(k)$$

**Top Row: energy band structures for four related models of Chern Insulators. Note which are delocalized.**

**Bottom Row: Berry Curvatures for the structures. The Chern numbers are $0, 1, -1,$ and $0$ respectively.**



## Critical Exponents and Phase Transitions

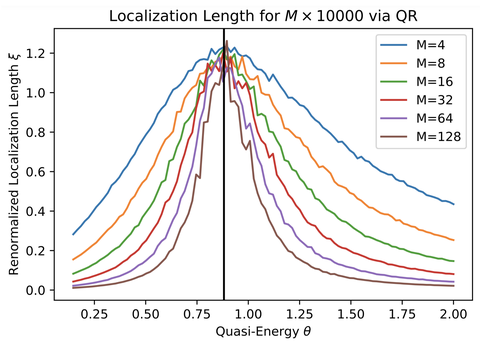
The localization length, $\xi$, is defined by $\|\psi\| \sim \exp(|x - x_0|/\xi)$, where the decaying exponential bounds the wavefunction. The localization length may be found from transfer matrices $\mathcal{T}$, by $QR$-factorization, using the method of Lyapunov Exponents:

$$\prod_{l=1}^{L}\mathcal{T}_l = Q_L\prod_{l=1}^{L}R_l; \qquad \gamma_l = \ln|R_l(1,1)|; \qquad \gamma = \frac{1}{L}\sum_{l=0}^{L}\gamma_l; \qquad \xi = \frac{1}{|\gamma|}$$

The critical exponent for may be found at the critical point:

$$\xi\big|_{M=\infty}^{\theta\sim\theta_c}(\theta) \propto A|\theta - \theta_c|^{-\nu}$$

**Localization length for system widths $M$ in the Chalker-Coddington strip model. Interpolation finds a critical exponent of $\nu = 2.36$, in agreement with experiments and literature. Methods work for tight-binding models.**




## Conclusions

The Quantum Hall Effect provides valuable theoretical insights into our world, and serves as a model system to develop and test theoretical and numerical techniques. Here, computational modules were developed to numerically determine electronic band structures, berry curvatures, Chern numbers, localization lengths, and critical exponents for tight-binding and related models, with application to the Quantum Hall Effect. Results obtained were in good agreement with experiments and the literature.

Future research directions may include extending these methods and applying these modules to other models of electronic behavior, such as those of next-nearest neighbor interactions, higher Landau Levels, or to other systems such as Chern Insulators or Weyl Semimetals.

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