Butterflies and topological quantum numbers

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Abstract
The Hofstadter model illustrates the notion of topological quantum numbers and how they account for the quantization of the Hall conductance. It gives rise to colorful fractal diagrams of butterflies where the colors represent the topological quantum numbers.

1 The Hall effect in four acts
The first act in the Hall saga begins with a mistake made by James Clerk Maxwell, (1831-1879). In the first edition of his book “Treatise on Electricity and Magnetism”, which appeared in 1873, Maxwell discussed the deflection of a current carrying wire by a magnetic field. Maxwell then says: It must be carefully remembered that the mechanical force which urges a conductor ... acts, not on the electric current, but on the conductor which carries it. If the reader is puzzled that is OK, he should be.

In 1878 Edwin H. Hall was a student at Johns Hopkins University reading Maxwell for a class by Henry A. Rowland. Hall was puzzled by this passage and approached Rowland. Rowland told him that ...he doubted the truth of Maxwell statement and had sometimes before made a hasty experiment ... though without success. A schematic diagram of the scheme proposed by Rowland is shown in Fig. 1. Possibly, because of this failure, Hall made a fresh start, and tried to make accurate measurements of the changes in the resistance—a much harder experiment. This experiment failed, in accordance with Maxwell. Hall then decided to repeat the experiments made by Rowland, and following a suggestion of Rowland, replaced the original thick metal bar with a thin gold leaf and found that the magnetic field deflected the galvanometer needle. This work earned Hall a position at Harvard.

Maxwell died in the year that Hall’s paper came out. In the second edition of Maxwell’s book, which appeared posthumously in 1881, there is polite footnote by the editor saying: Mr. Hall has discovered that a steady magnetic field does slightly alter the distribution of currents in most conductors so that the statement in brackets must be regarded as only approximately true. It turned out that the magnitude, and even the sign of the Hall voltage depends on the conductor.
This made the Hall effect an important diagnostic tool. Maxwell, even in error, inspired a remarkable research direction.

The second act begins in 1929, with Werner Heisenberg and Rudolf Peierls. As we have mentioned above, the Hall voltage was found to be positive for some conductors and negative for others. One sign is “right”—it is what one would expect for (otherwise free) electrons moving under the combined action of mutually perpendicular electric and magnetic fields. The “wrong” sign was an embarrassment. It was as if the electrons had the wrong sign for their electric charge. The embarrassment was called the anomalous Hall effect.

Heisenberg, who pioneered the applications of quantum mechanics to condensed matter physics, suggested to Rudolf Peierls, who was his student at the time, to look into the problem of the anomalous Hall effect.

Peierls, building on the results of another student of Heisenberg, Felix Bloch, realized that the anomalous Hall effect could, indeed, be accounted for by quantum mechanics provided one takes into account the periodic crystalline field. Peierls showed that when the conduction band is only slightly full, the electrons behaved as if free, and the Hall response is consequently normal. However, when the conduction band is almost full the electron go the wrong way because of diffraction from the lattice. The conductance turns out to be determined by the missing electrons, i.e. the holes. The charge of a hole is opposite to the charge of an electron and this is how Peierls resolved the anomaly.

The third act begins in 1980 with Klaus von Klitzing discovery that the Hall conductance in certain two dimensional electronic systems, in suitable ranges of experimentally controllable parameters, is, to great accuracy, an integer multiple of $e^2/h = \left(25812.80727\,\Omega\right)^{-1}$. This discovery led to superior standards of resistance and to improvements in the determination of fundamental constants.

von-Klitzing was awarded the Nobel prize in 1985 for this discovery. The theoretical developments it spawned are wide and deep. In particular, it led to the identification of the Hall conductance with a topological invariant known as a Chern number. This scene from the third act is going to be our main theme.

The Hall effect has a fourth act, that of the fractional quantum Hall effect. It is no less dramatic, but, since it is not a story of topological quantum numbers, we do not tell it.

## 2 Surprising precision

The precise quantization of the Hall conductance raises a puzzle. The conductance of quantum dots is a sensitive fingerprint of the dot. Why rearrangements of even a few atoms in a dot have measurable consequences on the electric conductance, while in the quantum Hall effect, wildly different samples, manufactured in different labs, have precisely the same quantized values for their Hall conductance. The glib answer that the conductance of a quantum dot and Hall conductance of two dimensional electron gas are different, is correct, but not illuminating.

The integer Hall conductance is not only highly reproducible, it is also a
precise determination of a fundamental constant, $e^2/h$, ($e$ is the electron charge and $h$ is Planck constant). Why can a precision measurement of a fundamental constant be made on macroscopic systems that are incompletely characterized? Even more remarkable, why is the relation between the conductance and the fundamental constant, $e^2/h$, so simple?

It is instructive to contrast this state of affairs to the precision measurement of the (inverse) fine structure constant $\hbar c/e^2 = 137.03599976$. The latter is determined from measurements on the simplest system imaginable: a single isolated electron. Nevertheless, the relation between what is being measured and the fundamental constant $e^2/\hbar c$ is complicated. One measures the anomalous magnetic moment of the electron, $g_e + 2 = -0.0023193043737$, which, by quantum electrodynamics, can be expressed as a polynomial in $e^2/\hbar c$. The coefficients of this polynomial can be calculated in the theory of quantum electrodynamics. This is a difficult enterprise. The leading order of the polynomials had been calculated by Richard Feynman and Julian Schwinger in works that vindicated quantum electrodynamics and won them the Nobel prize in 1965. The higher orders necessary for precision determination require evaluating many integrals and relying on the help of computers.

In 1981 Robert Laughlin proposed a resolution of the puzzle. Here is a variant of his argument: Suppose one defines the conductance as the charge added to an electrometer when the time integral of the voltage equals the unit of quantum flux. By the principles of quantum mechanics each measurement of the charge on the electrometer yields an integer multiple of the electron charge. This quantizes the Hall conductance, simple because the number of the electrons that one can add to an electrometer is quantized.

There is a subtle gap in this argument: The charge on the electrometer is only a probabilistic quantity. Which integer will be found in any individual measurement depends probabilistically on the wave function of the system. The measured conductance is an average and hence need not be quantized.

To close the gap in the Laughlin argument one needs an additional argument why averages are also quantized. This is what topological quantum numbers do. In the context of the Hall effect the topological quantum numbers turn out to be the Chern numbers that arise in the theory of fiber bundles [6].

### 3 Topological quantum numbers

There are two distinct ways in which physical quantities get quantized. The familiar way one finds in textbooks of quantum mechanics is what we shall refer to as Heisenberg quantization. An example is the quantization of the charge, or the number of particles, that one finds on an electrometer. The theoretical reason for that is that in quantum mechanics observables are represented by matrices, and a measurement always yields an eigenvalue of the matrix. The operator associated with the number of particles on the electrometer has for its spectrum the set \{0, 1, 2, \ldots\}.

Topological quantum numbers are a more arcane form of quantization. The
mechanism is different from Heisenberg quantization. Dirac was the first to explore this avenue in his attempt to explain quantization of charge.

Dirac addressed the fact that nature seems to have a quantum of charge, so the ratio of the charges of two particles is always a rational number. For example, the charge of the proton is $-1$ times the charge of the electron. Not $-1.0001$. This is remarkable because the electron and proton are particles whose charges are not a-priori related in any obvious way. For example, their mass ratio is about 1836.109, which is not close to a simple fraction.

Dirac proposed a theory where the existence of a quantum of charge was an inevitable consequence of quantum mechanics. He showed that a magnetic monopole of charge $g$ forces the electric charge $e$ of any particle, to take value such that $\frac{2ge}{\hbar c}$ is integral. The existence of even a single monopole in the universe would therefore force all electric charges to be a multiple of one basic unit of charge. For various theoretical and experimental reasons, Dirac theory is not a completely satisfactory solution of the charge quantization problem, but it is a paradigm for an interesting mechanism for charge quantization and topological quantum numbers.

The Dirac argument for the quantization of the charge is not a consequence of the fact that the observable associated with the product $2ge/\hbar c$ is represented in quantum mechanics by a matrix with integer spectrum. In fact, $g$ and $e$ are treated as ordinary numerical parameters of the theory, not as matrices.

Here is one version of Dirac quantization argument. If one tries to write the vector potential for a magnetic monopole as a single function throughout space one finds a singularity on a string that terminates on the monopole. The string may be thought of as a thin solenoid that ends at the magnetic pole and feeds the magnetic flux. Now, if the flux carried by the string is an integral multiple of the quantum flux unit, the singularity of the vector potential can be removed by a gauge transformation. Since only the modulus of the wave function (rather than its phase) and the electromagnetic fields (rather than the potentials) have direct physical meaning, a singularity that can be gauge away is not a real singularity. The string is invisible to a quantum particle, and all that remains is the magnetic monopole. If, however, the flux is not an integer, the string can not be gauged away. It is real, and the monopole is just a pole of a semi-infinite solenoid.

The unobservable singularity of a Dirac string is like the coordinate singularity of the spherical coordinate at the north and south poles. The earth is perfectly smooth at the poles, but the coordinates fail to be smooth there with the mildly unpleasant consequence that there is no polar time zone.

That the Hall conductance is related to topological quantum numbers is an observation of David Thouless, Mahito Kohmoto, Peter Nightingale and Marcel den-Nijl [4]. They made this observation for two dimensional models of non-interacting electrons in periodic potentials. Interestingly, the topological aspects of these models were understood before in Boris A. Dubrovin and Serguei Novikov [5]. Novikov relates that he asked his colleagues at the Landau Institute what physical interpretation these invariants might have. Nobody gave him a useful suggestion. It was TKNN who, independently of Dubrovin and Novikov,
identified these topological quantum numbers with the Hall conductance.

The topological interpretation of the Hall conductance explains why the Hall conductance is not a fingerprint of the periodic potential. In Figs. 3, 5 this robustness can be seen from the fact that the colored regions are open sets. In particular, the Hall conductance does not change under small variations of magnetic field. The Hofstadter butterfly does not explain the quantization of the Hall conductance when electron-electron interaction is taken into account, nor does it explain the quantization when disorder is present. Both play a role in the real Hall effect. Much progress has been made in understanding these issues, [2, 8], but we shall not elaborate here.

4 Quantized averages

Are the topological quantum numbers, and Chern numbers in particular, really different from the ordinary quantum numbers one is used to in quantum mechanics? To appreciate the difference between ordinary quantum numbers and topological quantum numbers, we look at quantum expectations.

The number operator is quantized in the sense that an individual measurement of the number of particles in a given region always yields an integer. However, the quantum expectation of the number of particles need not be quantized. The quantum expectation is the value obtained by repeated measurements on identical systems. A peculiarity of quantum theory is that measurements are not strictly reproducible, because the theory is not deterministic but only probabilistic. As a consequence, even if the state of the system is precisely specified, the outcome of a measurement may yield different integers. Since the average of integers need not be an integer, the average value of the number of particles need not be quantized.

In the Dirac theory the quantization of the product $ge$ is more strict than Heisenberg quantization. Every measurement of $ge$ yields the same value, and not different multiples of a basic unit. In particular, both the individual measurement and the average are quantized and take the same value. Since both the individual measurement and the average are quantized the measurement is noiseless.

While the conventional Heisenberg quantization guarantees the quantization of an individual measurement, Dirac quantization, in the context of the Hall effect, guarantees the quantization of a quantum expectation value.

5 Hofstadter butterflies

Quantum mechanics seldom leads to colorful pictures. Perhaps one should expect this of a theory where rules for computing probabilities replace a mental image of reality. Hofstadter butterflies are among the few phenomena where quantum mechanics produces colorful, fractal pictures. Besides being pretty, the pictures also illustrate the concept of topological quantum numbers.
Hofstadter butterflies are Escher-like diagrams of infinitely many nested butterflies, flying to infinity. Their monochrome version, Fig. 4, was first described by Douglas Hofstadter in 1976, in his Ph.D. work under Gregory Wannier [7]. Hofstadter was fascinated by Mark Azbel's suggestion that under certain circumstances, the quantum mechanical energy spectrum of such systems can be a fractal set. Indeed, the self-similar character of the Hofstadter butterfly turned out to be closely related to the fractal nature of the spectrum (for irrational values of the magnetic flux). Interestingly, the history of the model that gives rise to the Hofstadter butterfly goes back to Peierls who proposed it as a thesis problem to P.G. Harper.

Neither Peierls nor Hofstadter considered the model in its relation to the Hall effect, but rather as a model with intriguing quantum mechanical spectral features. We shall take here the opposite point of view and will not consider here the spectral aspect of the butterfly at all. Instead we focus on the relation of the butterfly with the quantum Hall effect.

The colored butterfly diagrams, Figs. 3 and 5, describe the electronic phases of the quantum Hall effect. The colors represent quantized value of the Hall conductance. Warm colors (red) correspond to positive values for the Hall conductance, while cold colors (blue) correspond to negative values. White denotes vanishing Hall conductance. The quantized values of the Hall conductances were computed using the Diophantine equation of Thouless et. al. [4], (see box). Figs. 3 and 5 are the graphic expressions of this Diophantine equation.

Fig. 3 describes the situation where the magnetic field is the subdominant interaction. In this case, an external magnetic field will create gaps inside a crystalline energy band. When the Fermi energy is placed in a gaps the Hall conductance is an integer and the gap can be assigned a color. Figs. 3 shows the result of doing this for a large number of values for the magnetic field. The figure repeats periodically on this axis, with a period that is one unit of quantum flux $\hbar c/e$. This periodicity, is a version of Aharonov-Bohm periodicity. For natural crystals, where the unit cell has atomic dimensions and for the magnetic fields used in experiments on the Hall effect, the flux through a unit cell is at most of order $10^{-4}$ of the unit of quantum flux. This means that only a tiny sliver of the butterfly, near the bottom of the figure, is visible for natural crystals. A deeper exploration of the butterfly can, in principle, be achieved by growing super-lattices with large unit cells. The butterfly is flanked by white margins. The white margins mean that the Hall conductance vanishes if the (crystalline) band is either empty or completely full. This is what Peierls expected: Insulators should have vanishing Hall conductances.

Fig. 5 describes the situation when the magnetic field is the dominant interaction. In strong magnetic fields, the spectrum of the Schrödinger equation is a set of equally spaced points, known as Landau levels. A weak periodic potential will broaden each of the Landau levels into a set with gaps. Fig. 5 describes the Hall conductances when the Fermi energy is place in the gaps. Disregarding the colors, the butterfly then repeats periodically on the vertical axis, with a period that corresponds to adding a lattice cell.

Note that the color coding is not periodic and that while Fig. 5 has inversion...
symmetry, the butterflies in Fig. 5 do not have this symmetry. Note also that Fig. 3 has no albino butterflies, while Fig. 5 does. This is one way to see that the two figures represent different systems.

The butterfly of a broadened Landau band is an experimental challenge because of conflicting experimental requirements [11] which were only recently overcome in Albrecht et. al. [11].

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7 Box: Nuts and bolts

This box is for the reader who would like to write his own computer program to make colored butterflies. Further information can be found in [12].

There are two steps involved. The first step is an eigenvalue problem that determine the boundaries of the wings of the butterfly. The second step is to solve a number theoretic problem that determines an integer for each wing. This integer is used to color the wing. Let us briefly outline these two steps.

The first step is to solve for the eigenvalues of a quantum Hamiltonian describing the dynamics of an electron in two dimensions. Using the symmetry of the problem, the two dimensional Hamiltonian can be reduced to the study of a one dimensional eigenvalues problem commonly known as the Harper equation

\[ \psi(n+1) + \psi(n-1) + 2 \cos(2\pi \Phi n) \psi(n) = E \psi(n) \] (1)

\( E \) is the requisite eigenvalue. In the tight binding limit, \( \Phi \) is the flux through a unit cell (in natural units). In the limit of split Landau band, \( \Phi \) is the inverse of the flux through a unit cell.

There are no effective ways to solve this eigenvalue problem when \( \Phi \) is irrational. However, for \( \Phi = \frac{p}{q} \) one looks for periodic and antiperiodic solutions:

\[ \psi(n+q) = \pm \psi(n) \] (2)

The corresponding eigenvalues are then determined by two, essentially tri-diagonal, \( q \times q \) matrices. The \( q \) eigenvalues of the periodic solution determine half the edges of the wings for that value of \( \Phi \) and the other half come from the corresponding anti-periodic solutions.

It remains to associate a color with each band gap. The algorithm described below is built on the original algorithm of [4].

Suppose that the magnetic flux through a unit cell is \( \frac{p}{q} \). For \( p \) and \( q \) relatively prime, define the conjugate pair \( (m, n) \) as the solutions of

\[ pm - qn = 1 \] (2)

\( m \) is determined by this equation modulo \( p \) and \( n \) modulo \( q \). The algorithm for solving Eq. (2) is one of the oldest in mathematics: A division algorithm of
Euclid. (Standard computer packages for finding the greatest common divisor of p and q, yield also m and n such that \( pm + qn = \gcd(p, q) \).) The Hall conductance \( k_j \), associated with the j-th gap, in the tight binding case, is given by

\[
k_j = jm \mod q, \quad |k_j| \leq q/2
\]

In the case of split Landau band, Eq. (3) again determines \( k_j \) provided \( p \) and \( q \) are interchanged.

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Figure 1: A schematics of the experimental setup of the Hall effect. A current driven through the conductor, drawn as a prism, leads to the emergence of voltage in the perpendicular direction. This is the Hall voltage, which Maxwell erroneously predicted to be zero.

Figure 2: The vector potential of a monopole is singular on a string. When the string carries an integer number of flux quanta it can be gauged away.

Figure 3: Colored Hofstadter butterfly for Bloch band split by magnetic field. The horizontal axis is the energy, or the chemical potential; the vertical axis is the magnetic flux through the unit cell in natural units.

Figure 4: The original, monochrome, Hofstadter butterfly, describes the spectrum of a quantum particle in a magnetic field and periodic potential. The vertical axis is related to the magnetic field, and the horizontal axis is the energy axis.

Figure 5: Colored Hofstadter butterfly for a single Landau level split by a periodic potential. The horizontal axis is the energy, or the chemical potential, the vertical axis is the inverse of the magnetic flux through the unit cell in natural units.
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