# TOPOLOGICAL QUANTUM MATERIALS

## From Theory to Simulation


Made by: Bru Serra, Marcel Vilaró, Stefan Giurgiu

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# 1.Introduction

## 1.1. General context

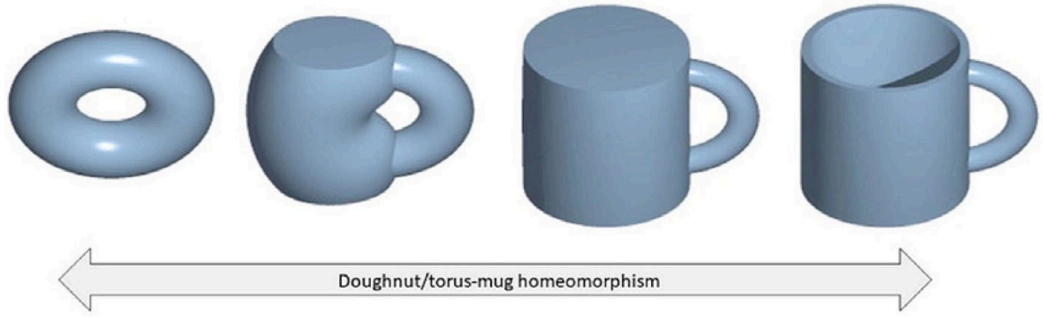
We are in Physics, a broad field of pure science study. To get our eyes where we want, we must first zoom in on modern physics, which englobes the discoveries from the 1900 onwards. The field we are interested in is condensed matter physics, that stems from statistical mechanics and quantum mechanics. It studies the behavior of large numbers of particles (mainly electrons) in solids and liquids. Now, taking one step further into the tree that represents the diverse disciplines of physics, we arrive at the field of topological quantum materials.

The goal of this work is to give some insights into this field, covering mainly quantum insulators through the study of diverse quantized Hall Effects, both theoretically and practically via a computer-based condensed matter simulation, and then its applications with Majorana Qubits.

## 1.2. Mathematical Topology

Topology is quite a recent branch of mathematics, with most of its discoveries and studies being done around the 1900s by renowned mathematicians such as Poincaré, Riemann or Möbius. However, its origins date back to the year 1735 with the famous problem of the Könnigsberg bridges, posed by Leonhard Euler, in an attempt to cross all seven of them without retracing his steps.

This apparently abstract field mainly studies spaces that remain invariant to continuous deformations, in other words, that behave like “rubber objects”. They can be stretched, twisted,... but never perforated or “glued”, the number of holes is a constant of each object. The most popular example of this is the doughnut-mug analogy, to the eyes of a topologist, both are identical, since they can be continuously morphed into the other.



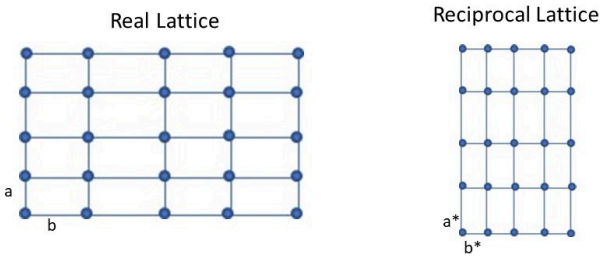

Technically speaking it is said that for two spaces to be topologically equivalent they must be homeomorphic, which means that there is a continuous bijective application that goes from one space to the other. Despite generally referring to holes as the characteristic element of these spaces, we can also consider the crossing of strings

in a knot or the number of windings of a periodic wave function, being this last example the most interesting in the context of quantum physics.

In addition, of the four principal topological subfields of study, the most contributing one in this project will be algebraic topology since it allows to view complex topological problems as simpler algebraic ones considering the global properties of spaces.

## 1.3. Topological Quantum Materials

The key idea behind topological quantum materials is that their behavior is given by a constant invariant to smooth changes, in other words, the topology is the principal characteristic. Despite having several impurities or imperfections, the result will be the same as long as the wave function has the same topology. This property is observed inside the so-called brillouin zone, which is the Voronoi cell of each point of the reciprocal lattice. Interestingly, this new reciprocal space emerges from taking the fourier series of the potential and imposing periodicity conditions.

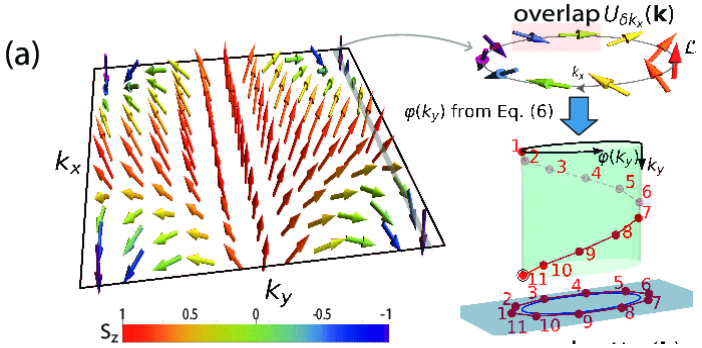



In this region the wave function is not periodic and constitutes the unitary cell for the wavefunction of the whole lattice[1].

Due to this periodicity and the continuity of the wavefunction we can impose the restriction that it (the function) must be equal in opposite sides. It can be understood as if the wavefunction was in a toroidal space, where going off one limit returns you to the other one.


[1] Result of the Bloch Theorem, which will be briefly covered later.

Because of this, we can now define a topology inside that region, if the wave function has a twist or a *winding* there is no such continuous transformation that allows it to be untwisted, meaning that, as previously mentioned, it is a topological characteristic.




# 2.Topological Insulators

## 2.1. Band Theory

Band theory is a fundamental concept in condensed matter physics that we need to be familiar with in order to grasp even the slightest understanding about the topic of this work. Therefore, some non-trivial explanation must be done on the subject.

### 2.1.1. Paul drude model:

The antecedent of band theory would be the Paul Drüde model (1900), which stated that solids where a mixture of positively charged nuclei together with the inner shell electrons, 'cations' called altogether, and unbounded electrons from the outer shells of the atoms, called the 'free electron gas'. Although this model explained thermal conductivity, it couldn't properly explain the fact that some materials were conductors and others were insulators.

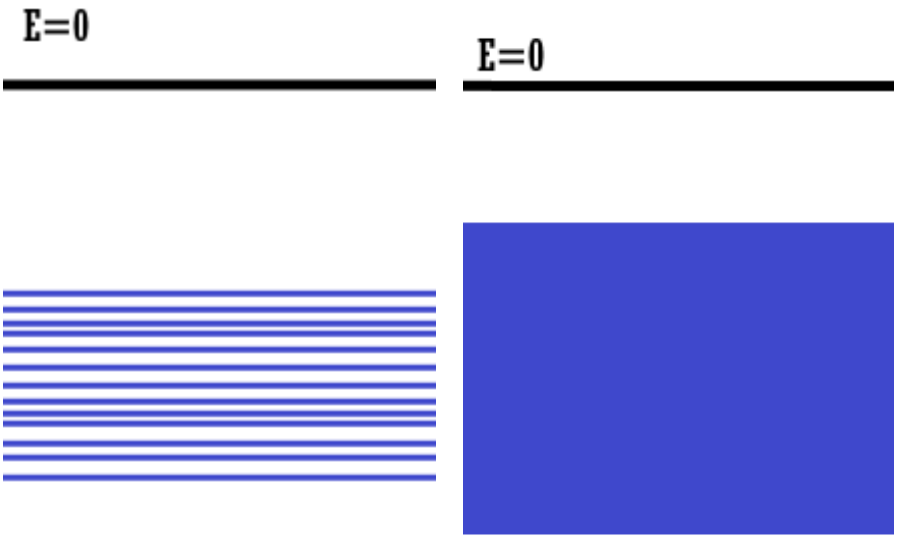
In 1928 Felix Bloch, became Werner Heisenberg's first graduate student and got his Doctorate at the age of 23 years. In his thesis, he explored the effects of quantum mechanics in solids.
He assumed atoms arranged in an array (called crystal) and applied the Schrodinger equation to the system. This was a radically different problem than considering a single atom in a gas, as the conditions were nothing similar. What he got is a solution for the valence electrons (outermost shell electrons) that is known as Bloch's theorem.

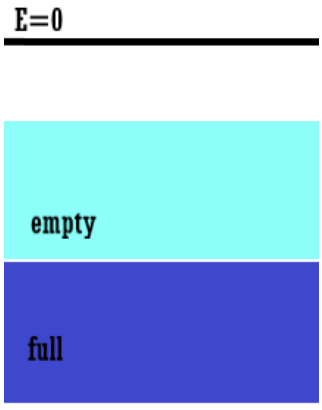
$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$$

Where **k** (crystal momentum) is directly related with the wave number of a plain wave and lies in the aforementioned reciprocal lattice. This also implies that all relevant physical information is contained in such reciprocal space, often labeled as **k-space**. $u(r)$ is a function with the periodicity of the bravais lattice.

This solution is periodic and it says that only certain wavelengths are permitted for the electrons in a crystal, which correspond to states where electrons can move freely through the lattice, giving rise to conduction. This also obviously means that there are some forbidden values of energy for the electrons.
Bloch, who would later get a nobel prize for works in the field of nuclear physics, had laid the groundwork for other physicists to build upon.

Lets now look into the work of Walter Heitler and Fritz London (the same guy from the London forces). They used the theory of LCAO-OM (Linear Combination of Atomic Orbitals - Molecular Orbitals) with large aggregates (solids). Think about the 1s orbital of the hydrogen atom. When two hydrogen atoms combine, a lower-energy, bonding orbital and a higher energy, antibonding orbital arise. Now let's consider we have $10^{21}$ atoms of gold, which is about a gram. Due to conservation of states, when we combine their orbitals (considering the outer shell s1 orbitals) we should have the same number of states as atoms. If we plot each state as a horizontal line, the energy in the y-axis, we would be seeing so many lines that they would appear continuous, just like a **band**.




As a numerical example, we can approximate the lowest state energy of gold by $\simeq 10e\,V$, so we see the $\Delta E$ between different states would be about $10^{-20}eV = 1.6 \cdot 10^{-39}J$, which is really small.
If we now try to fill this band, it will stay half empty, as the gold outermost shell only has one 's' electron. The difference of energy from the empty band and the full band (conduction and valence band respectively, from now on) is, for our example, precisely $10^{-20}eV$ (and is called energy gap). For reference, $0.025eV$ corresponds to $290\,K$ which is about room temperature. Therefore electrons can very easily jump

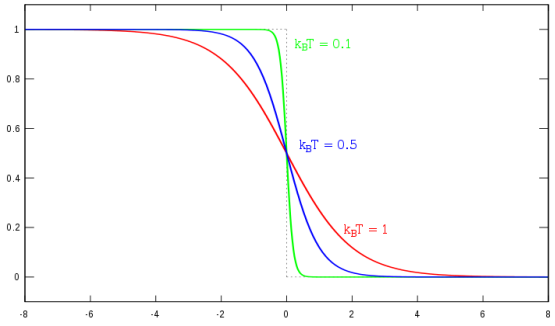
to the empty states under some potential applied, leading to conduction. Thus gold is a metal (actually the metal with the third lowest resistivity).
If we now were to do this very same procedure with different materials, we would see that some have a noticeable energy gap.
This leads to the classification of materials we all know:

- Conductors (metals): The valence and conduction bands are overlapped, with no energy gap between them.
- Insulators: Large energy gap between valence and conduction bands.
- Semiconductors: Narrow energy gaps.

Insulators usually have an energy gap greater than $4\ eV$ and semiconductors have one lower than $1.3\ eV$. Take visible light as reference, which is about $1\ eV$.

### 2.1.2. The Fermi level

For what concerns us, the Fermi Level is *the energy level which would have a 50% probability of being occupied by an electron at any given time* (at thermodynamic equilibrium). Note it can also lie within the band gap, so it doesn't imply that an electron can *actually* have that energy.
The Fermi level basically provides us with a reference energy that tells us how electrons would distribute if all energy levels were available, and thus represents how easily a material can conduct electricity.




This graph shows the Fermi-Dirac distribution. In the *y-axis* is the probability that given energy level, or state, (*x-axis*)[2] is occupied by a fermion (e.g., electron). E=0 would represent the Fermi Level. We see that the higher the temperature, the higher the probability for electrons to be found higher than the energy level, and thus to conduct current.

## 2.2. Quantum Hall Effect

### 2.2.1. The Integer Quantum Hall Effect (IQHE)

Although the Hall effect seemed fully characterized, in 1980 von Klitzing's experiment demonstrated that there was still much to discover. Klaus von Klitzing was investigating the transport properties of two-dimensional electron gases in silicon at very low temperatures (1.5 Kelvin) and under strong magnetic fields (18 Teslas). According to the classical theory proposed by Hall, he expected to see a straight line when plotting the Hall resistance against the magnetic field B.

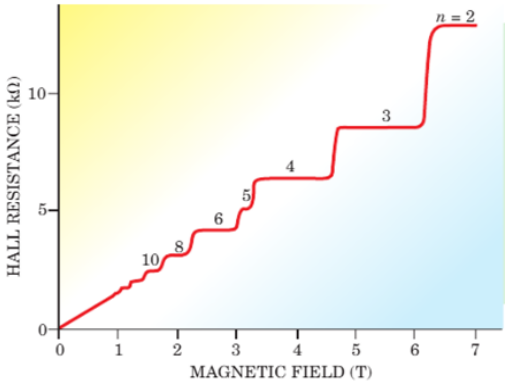
[2] The energy is actually normalized by the chemical potential and centered, so the fermi level lies at 0.

However, he found a surprise when, unexpectedly, the Hall resistance presented a series of perfectly flat steps instead of a smooth straight line. In these steps, the resistance value did not change at all as the magnetic field varied.

The resistance values fitted perfectly with the formula:

$$\rho_{xy} = \frac{h}{e^2}\frac{1}{v}$$

Where h is Planck's constant, e is the charge of an electron, and v is an exact integer (1, 2, 3, …). This effect, called the Integer Quantum Hall Effect (IQHE), demonstrated that Hall conductance was quantized. The precision was very good, regardless of material imperfections, geometry, or the purity of the silicon.




To understand this effect deeply and give it an explanation from quantum physics, we must abandon classical dynamics and think about the quantum mechanics of an electron in a magnetic field. As we already know, in a magnetic field an electron performs circular orbits, and the orbit's energy can vary according to the radius (and therefore also according to the speed).

In the quantum world, there are restrictions; the wave function that results from solving the Schrödinger equation for the system collapses into discrete energy levels, called Landau Levels.

The energy of these is given by:

$$E_n = \hbar w_c (n + 1/2)$$

Where n = 0, 1, 2, …. are the Landau levels.

Each of these levels is highly degenerate (it can contain many electrons). Relating this to the quantum Hall effect formula, the integer number "v" appearing in von Klitzing's formula is physically interpreted as the Filling Factor: the number of Landau levels that are completely occupied by electrons.

When the magnetic field B is adjusted so that an integer number of Landau levels are full and the upper ones are empty, an energy gap opens between the highest occupied state and the lowest empty state. When this happens, the system behaves like an insulator in its interior, since a finite amount of energy is needed to excite an electron to the next level.

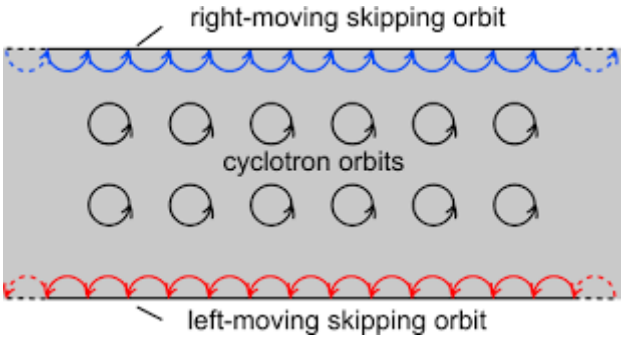
But there is still a fundamental question. We now know that Hall resistance should take quantized values only at precise points of the magnetic field (offering us a graph where we would have something like Dirac deltas at these points), but contrary to what we think, these values remain constant while the magnetic field changes.

And here lies the irony of solid state physics: the perfection of quantization requires the imperfection of the material. In an ideal sample, it would behave like a series of deltas plotted at certain moments. But since real samples contain impurities, defects, and disorder, the perfect degeneracy of Landau levels is broken, widening them into energy "bands".

Although there are still many questions to resolve, such as: how does the current flow if the interior is insulating?

To answer this, we must look at the edges of the sample. In the interior ("bulk"), electrons perform closed orbits and there is no net displacement of charge, but electrons at the physical edge cannot complete their circle; they hit the potential barrier of the edge and bounce off. Since the magnetic field continues to act, the electron is forced to curve back towards the edge, bouncing repeatedly.

The result is a trajectory that resembles a series of hops along the perimeter of the sample, known as a "skipping orbit". And if we define that, for example, the direction of rotation on the upper edge is to the right, on the lower edge it will be forced to the left.




This unidirectionality protects the current: if the electron encounters an impurity at the edge, it cannot bounce back; it simply goes around it and keeps moving forward. This results in zero longitudinal resistance and perfect conductance.

### 2.2.2. Topological view

The explanation given by Landau levels is satisfactory but still did not explain why details like the shape of the sample did not affect it. In 1982, TKNN revealed that the quantization of Hall conductivity is a manifestation of the topology of the quantum state space.

To explain this, we must introduce the concept of the Berry Phase. As we already know, in quantum physics, the wave function has an amplitude and a phase. Usually, the phase was not given much importance, but in 1984 Michael Berry demonstrated that when a quantum system evolves adiabatically (slowly) along a closed path in parameter space, it acquires an additional phase that is fundamentally geometric.

In the band structure of a solid, the "parameter space" is the Brillouin Zone, the set of all possible crystal momenta "k". Due to the periodicity of the crystal lattice, the Brillouin Zone has the topology of a torus, as we previously mentioned (leaving through one side k = π means re-entering through the opposite side k = - π).

TKNN applied perturbation theory to calculate the Hall conductivity of a periodic 2D system in a magnetic field. They found that Hall conductivity could be expressed as an integral over the entire Brillouin Zone:

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi i}\int_{ZB} d^2kF(k)$$

Where F(k) is the Berry curvature, a fictitious vector field that describes how the energy band eigenstates "twist" as we move in the momentum space “k”.

And here we find the magic: the integral of the Berry curvature over a closed surface is a topological invariant. The quantity $C = \frac{1}{2\pi i}\int_{ZB} d^2kF(k)$ is actually an integer. This number is described as the Chern Number.

Therefore, Hall conductivity can be rewritten as $\sigma_{xy} = \frac{e^2}{h}C$ where C is the sum of the Chern numbers of all occupied bands.

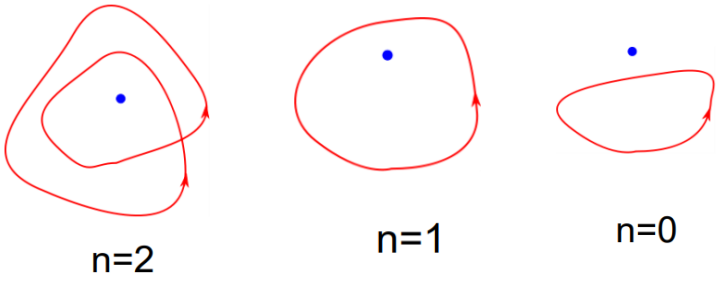
### 2.2.3. Chern Number

The need for topology arose when studying the quantum hall effect. Even though really insightful, the results obtained led to a typical band structure for the energies, no different from a regular insulator. Thus something new ought to be introduced that could differentiate the two, pole apart, different states. This something new was the Chern number, which borrowed the aforementioned topological concepts and

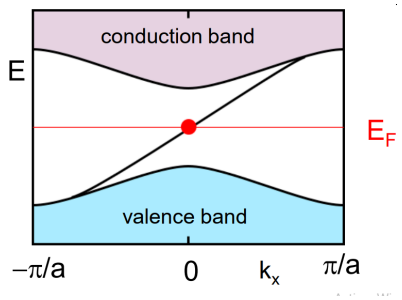
properties, namely the invariance to smooth changes. It was then proven to precisely correspond to the 'integer' quantizing the conductivity of the quantum hall effect.

$$n = \frac{1}{2\pi i}\int_{BZ} d^2\mathbf{k}\cdot\left\langle \nabla_{\mathbf{k}} u(\mathbf{k})\right| \times \left|\nabla_{\mathbf{k}} u(\mathbf{k})\right\rangle \in \mathbb{Z}$$ u(**k**) = Bloch wavefunction

The Chern number characterizes the quantized hall conductivity: n=0 would correspond to an insulator(with zero conductivity). It can also be thought as a winding number, that counts the curve's number of turns around a point:

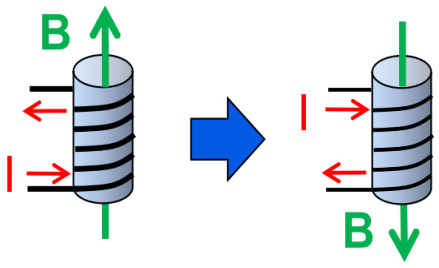



Looking at band diagrams, n would indicate the number of conducting states at the edges, which you can think of as electron VIP (meaning only for the electrons in the edges, not for the ones in the bulk) highways to the conduction zone. The bigger the n, the more highways in which electrons can be, thus more traffic of electrons to the conduction zone and so higher conductivity (this has a caveat: it also depends on the chirality of the states). Moreover, the conduction of electrons along the edge is perfect, without dissipation. This happens because the edge states move only in one direction so they cannot backscatter. Entering again the analogy, you can think that electrons are not allowed to turn back on the highway, so all of them are conducting. If some electrons were to travel in the opposite direction, the conductivity would be lower for the same number of electrons. Due to the topological properties electrons will keep flowing even if you modify the route of the highway (homeomorphic transformation). They would stop flowing if you destroyed a part of the highway (change in topology).



## 2.3. Time Reversal Symmetry

Another key concept to understanding the differences between different topological quantum materials is time reversal symmetry (TRS).
This concept basically describes how physical systems behave when the direction of time is reversed. If a system does have TRS, then when time t is replaced by -t physical laws remain unaltered. Here's an example:



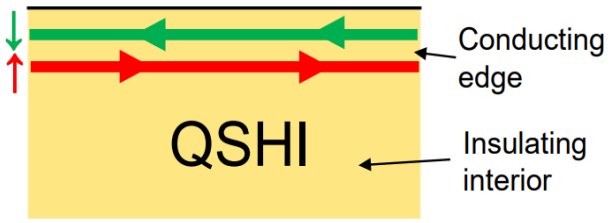

- Magnetic field: When we reverse time, current flows in the opposite direction, and by the right-hand rule the induced magnetic field also changes direction. The system has changed, therefore it **doesn't** have TRS (it *breaks* TRS).
- The Quantum Hall effect ***breaks*** TRS

Now one could ponder whether topological phases exist with *unbroken* TRS. The answer is *yes*.

## 2.4. Quantum Spin Hall Insulator

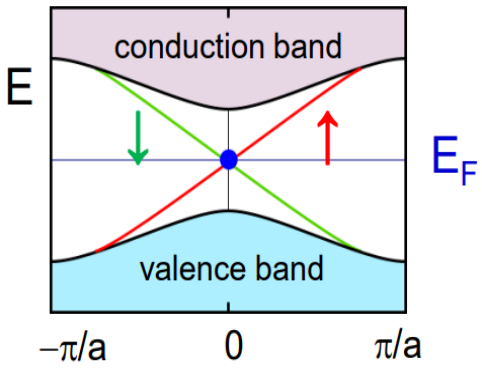
In 2006 Bernevig and Zhang published a paper in the science journal in which they predicted the existence of a new topological state of matter in absence of a magnetic field. They called it the *Quantum Spin Hall Effect* (BHZ model). A year later König et al did an experiment[3] (also published in the Science journal) based on the suggestions of the 2006 paper in which the existence of such an effect in HgTe/CdTe quantum wells was confirmed. This was a huge success of the topological quantum band theory.

The quantum spin hall (QSH) state is a topological phase of matter in which the bulk of the material is insulating and has conducting edge states that carry spin currents without a net charge current (gapless helical edge states). This means that spin up electrons will all move along the edge in one direction (lets say rightwards) and spin down electrons will all move in the **opposite** direction. The result is zero net transportation of charge (net current) because both currents 'cancel' each other. These states **are** protected by TRS. If we were to change *t* by *-t* spin up electrons would travel leftwards (in this example), and spin down rightwards. This 'new' state is equivalent to the one we had before, so TRS has not been broken.




Moreover, the QSH conductance is **quantized** in units related to spin.

[3] which will later be explained

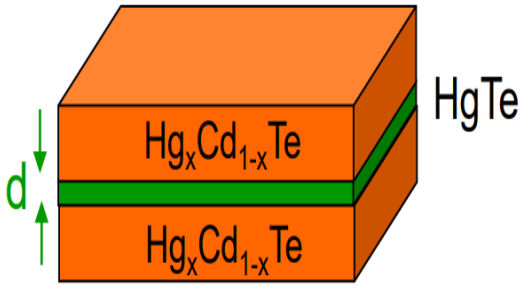



In this band diagram we can observe the two edge states, one for each spin.
You can easily think about the highway analogy again considering two different highways which lead in opposite directions.
Because of TRS, transport of electrons in the edges is dissipationless. This is because TRS doesn't allow backscattering. In terms of our analogy, we can think that the highways for different spins never intersect, so there is no danger of electrons frontally colliding and dissipating energy.

Note that this effect happens in the absence of a magnetic field and is topologically protected by **nonmagnetic** impurities.

### 2.4.1. Experiment on HgTe/(Hg,Cd)Te quantum wells

HgTe/(Hg,Cd)Te quantum wells are made by sandwiching a thin layer of mercury telluride (HgTe) between layers of an alloy, mercury cadmium telluride (Hg1−xCdxTe). The use of this specific materials is not by chance, as it corresponds to a careful 'band engineering' based on relativistic effects. In the majority of conductors of group II-VI the conduction band (s type symmetry) is energetically **over** the valence band (p type symmetry).




So, while Hg1−xCdxTe has a normal semiconductor band structure, HgTe is a zero/negative gap semiconductor. This is because it had an *inverted band ordering*, meaning the valence band states are **higher** in energy than the conduction band states. It is worth noting that this is due to relativistic corrections on the electron orbits close to the heavy mercury nuclei.

When assembling such 'sandwich structure', the effective electronic structure depends critically on the *thickness*, *d*, of the HgTe layer.
What was found in the experiment is that when *d<6.3 nm* the quantum confinement raises the energy of the 'well' states(in HgTe), reverting the inversion and getting a normal band structure, so the system behaves like a normal insulator. However, when *d>6.3 nm*, the inverted band ordering 'survives' the confinement, letting rise to the topological regime. Meaning the '2D' system becomes a QSH insulator (QSHI) with helical edge states. This observed phenomenon is called a *quantum phase*

*transition* (by crossing *6.3 nm*, the critical thickness). Moreover, the edge conductance was also measured to be independent of the sample width, providing the final evidence of the existence of the QSH effect.

## 2.5. Topological Classification ($Z_2$ Invariant)

Historically, the theoretical foundation for the phenomena described above was laid by Kane and Mele in 2005, a year before the BHZ proposal. They demonstrated that intrinsic spin-orbit coupling (SOC) could act as an effective magnetic field, generating a topological phase while preserving TRS.

Kane and Mele realized standard topological classification wasn't too accurate. To solve this, they introduced the $Z_2$ topological invariant ($v$). This new binary index provided the mathematical framework to distinguish strictly between a trivial insulator ($v = 0$) and the Topological Insulator ($v = 1$) observed later in the HgTe experiments.

# 3.Topological Qubits

## 3.1. Majorana Fermions

Beyond the previous examples of effects without apparent everyday use, resides an idea that proved to be possible would result in a major breakthrough on quantum technologies. We are talking about topological qubits, precisely about those based on Majorana Modes, a new type of qubit that would allow quantum computers orders of magnitude more powerful and reliable than the current ones.

In order to understand the functioning of these qubits we must start explaining the core idea, Majorana Fermions.
In particle physics all particles are divided into two groups, fermions and bosons, the first ones have the property of half-integer spin and obey the Pauli exclusion principle, bosons have integer spin and do not obey Pauli's principle. The ones we are interested in, fermions, in the vast majority of cases, like with all of the elemental fermions the particle is not its antiparticle, this means that given two identical Dirac fermions, they would not annihilate each other. However, when repeating the experiment with now majorana fermions, the result is the opposite, meaning that each particle is its own antiparticle.

This behaviour can be justified mathematically by considering a real defined wave-function so that when conjugated it remains the same. Because of this the mathematical operators of creation an annihilation ($\gamma^\dagger$, $\gamma$ respectively) for majorana fermions are also equal.

$$\gamma^\dagger = \gamma \quad c^\dagger \neq c$$

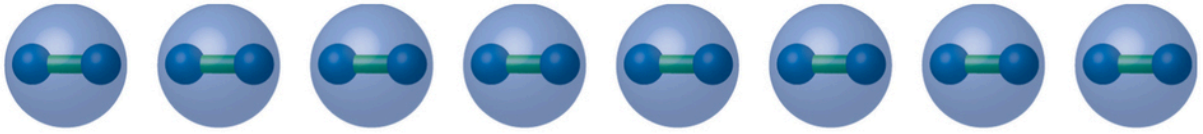
Despite having so much knowledge about these fermions, they have not been observed yet, although experimental results do not deny its existence. A very good candidate for the moment are a particular type of neutrinos that would participate in double beta decay without neutrino emission, but sadly there is no evidence that it happens. However, in condensed matter physics there is another option which is the one we are interested in, a majorana quasi-particle.

In condensed matter physics a quasi-particle is a disturbance in a medium that can be localised and behaves just like a regular particle, having charge, spin, momentum and many other properties, despite not being able to exist by itself.

A quite common quasi-particle are electron holes in crystal lattices. If the valence band of all atoms in a crystal is full, after promoting an electron to the conduction band, where it used to be there is now a “hole” that can be filled by other neighboring electrons. When this happens the electron that has filled the original hole leaves behind a new hole, just as if it had moved. This hole behaves like the antiparticle of the electron since they mutually annihilate and considering the global charge of the crystal they must have opposite charges. If initially an atom is neutral, creating a pair hole-electron (exciting one electron out of the atom) must conserve the charge, the electron and the hole must have the same charge but with different signs.

## 3.2. Kitaev Chain

This idea comes very useful when analyzing the behaviour of a Kitaev chain.
A kitaev chain is the modelization of electrons in a superconductor wire. Since they move uniformly (in Cooper pairs) and without scattering, the number of electrons inside of the cable is constant, the Kitaev chain is when we consider the electrons of this system in fixed positions and in a discrete distribution with aligned spin. Just as if we were taking photos of the system periodically.



Since we said previously that majorana fermions are their own antiparticle we can describe the wave function (ψ) of, for example, electrons as the addition of the wave functions of two Majorana fermions, which from now on will be called α and β.

$$\alpha(x) = \psi^{\dagger}(x) + \psi(x) = \alpha^{\dagger}(x)$$

$$\beta(x) = i(\psi^{\dagger}(x) - \psi(x)) = \beta^{\dagger}(x)$$

$$\psi(x) = \frac{1}{2}(\alpha(x) + i\beta(x))$$

α will be the majorana fermion that corresponds to the real part of the electron's wave function, and β to the imaginary part. Combined they form the wave function of the electron. If we now calculate the hamiltonian of the system of N electrons we get the following expression:

$$H = \sum_{n=1}^{N-1} (\Delta \psi_n^\dagger \psi_{n+1}^\dagger + t\psi_n^\dagger \psi_{n+1} + h.c.) - \mu \psi_n^\dagger \psi_n$$

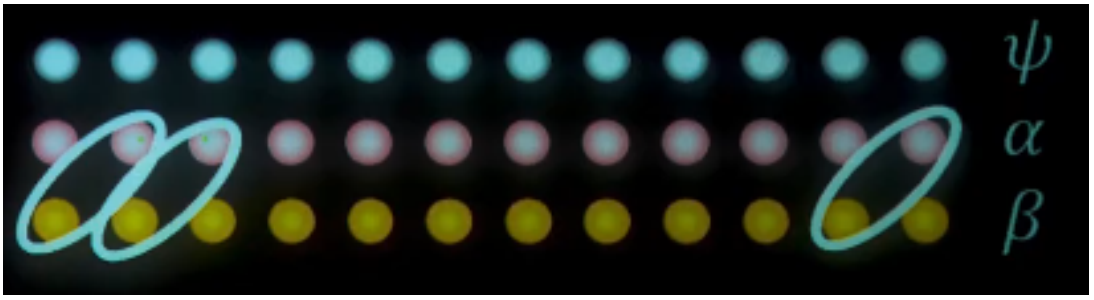
The first term of the sum corresponds to the pairing of electrons due to superconductivity, the second corresponds to the hopping term (annihilation of an electron in a position and creation in the next one) and h.c. is the Hermitian Conjugate, put there to ensure the energies are real and not imaginary.

In this equation μ and t can take many values, but if we strategically choose t=Δ and μ=0 (meaning that the hopping parameter is equal to the Cooper pair energy, and the chemical potential is 0) we can solve the equation much more easily getting to this hamiltonian:

$$H = \sum_{n=1}^{N-1} \Delta \left| (\psi_n^\dagger - \psi_n)(\psi_{n+1}^\dagger + \psi_{n+1}) \right| = \sum_{n=1}^{N-1} \Delta \left| i \frac{(\psi_n^\dagger - \psi_n)}{i} (\psi_{n+1}^\dagger + \psi_{n+1}) \right| =$$

$$= - \sum_{n=1}^{N-1} i\Delta \beta_n \alpha_{n+1} = \sum_{n=1}^{N-1} i\Delta \alpha_{n+1} \beta_n$$

Multiplying and dividing by i we get -β, so we can substitute both terms by β and α and then applying the anticommutative property of Majorana fermions we get a very interesting equation. This can be interpreted as the energy of the Kitaev chain depends on all α fermions except the first one, and all the β fermions except the last one. This is due to the fact that the system can be understood as majorana fermions interacting "in diagonal".




In other words, we define a new fermion quasiparticle that has this wave function:

$$f_n = \frac{1}{2} (\alpha_{n+1} \beta_n)$$

instead of $\psi_n = \frac{1}{2}(\alpha_n + i\beta_n)$ like the original electrons.

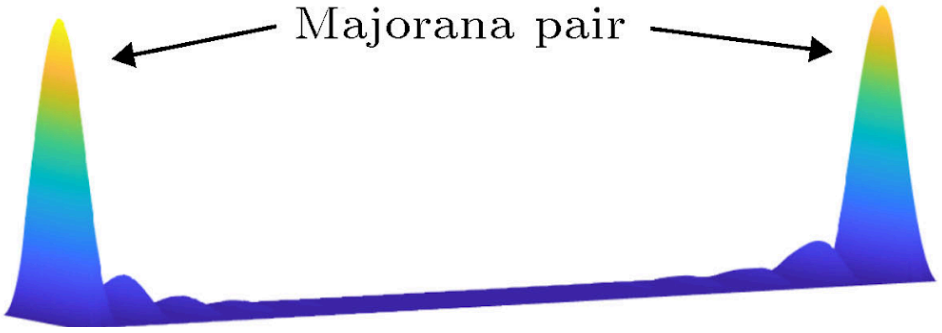
Since the number of electrons must be equal to the number of "f" fermions we must define another fermion that includes the first left out α and the last β.

$$f_N = \frac{1}{2}(\alpha_1 \beta_N)$$

This is what we call the Majorana zero mode, a quasi particle that has E=0 because of that previously mentioned about the contribution to the hamiltonian of $\alpha_1$ and $\beta_N$.

## 3.3. Majorana Zero Modes

This fermion has a very strange wave function, due to the fact that "it is split" in two halves, the wave function has two peaks, one at each end of the kitaev chain, or in other words, has radically different behaviour on the edges.




This delocalized nature of the wave function is a topological property and doesn't change under the influence of electromagnetic fields or by elongating or shortening the wire.

Because of this in order to alter the wave function, both peaks must be affected simultaneously, which is quite unlikely compared to localised wave functions. It should also be taken into account that the longer the chain, the more delocalized the wave function is, and thus more stable.

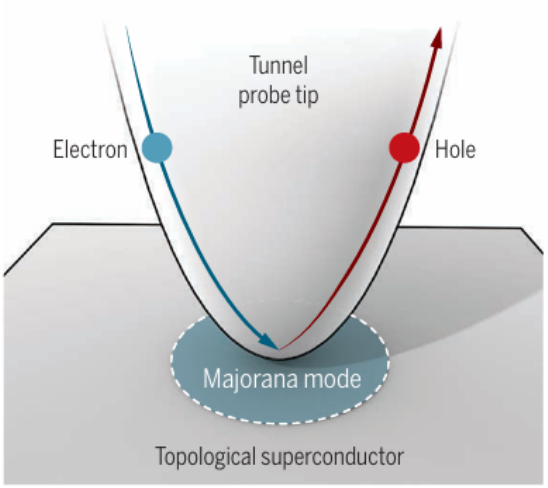
However, Majorana Zero Modes (MZM) could appear in a wide variety of situations, for example, in Fractionary Quantum Hall effect, where the system would be more robust, or in topological superconductors, which enable easier state measurements and are the most used ones in modern investigations.

## 3.4. Experiments with MZMs

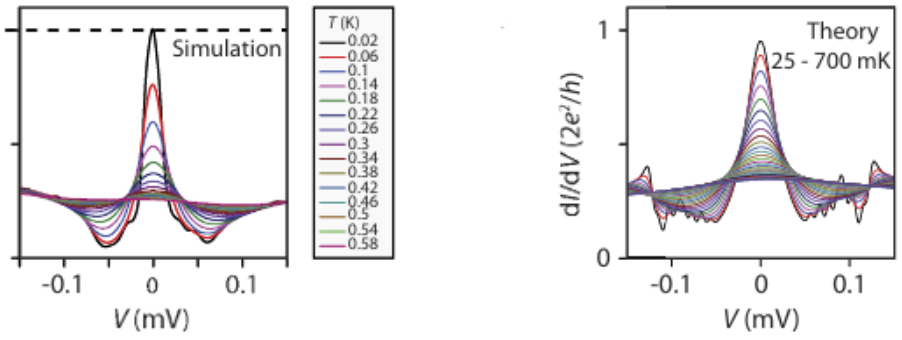
By taking a semiconductor (InAs or InSb) nanowire covered by a superconductor, we get a topological superconductor which can hold MZMs. This is due to the fact that

those semiconductors have very strong spin-orbit coupling and enable the system to fulfill the Kitaev conditions.

If we now take this superconductor and place a sharp probe close to it, after applying a very small voltage we can test whether there are or not MZMs. In the presence of MZMs it will be possible to add an electron via tunneling into the wire, this mechanism is called Andreev reflection because when an electron leaves the probe a hole is reflected.



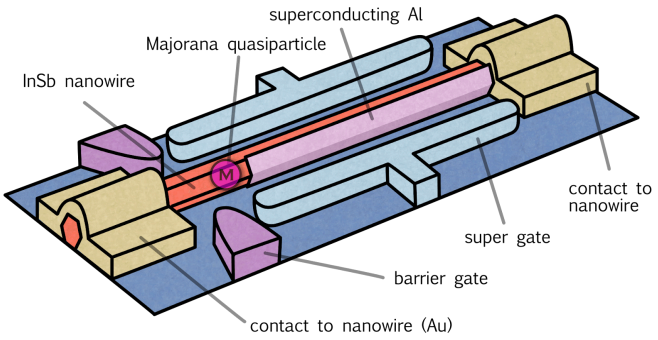

When MZMs are formed, if we apply a potential difference of the order of tens of microvolts we can observe a peak in the conductance up to $2e^2/h$ which contrasts heavily with the plateau observed for higher voltages. This happens because of the 0 energy of the wave function of MZMs, it constitutes a mid-gap band, so a new electron can only tunnel into the system if it also has very low energy.




This effect was thought to be observed experimentally in a recent investigation, however, further revision proved it to be just a bad analysis of the results, so for the moment we have no empirical evidence of MZMs existence, although we have neither found evidence of the opposite case.

In case of being proven to exist they could allow to build qubits based on whether an extra electron has been tunneled in or the MZMs are in the original state. Considering these are quantum states, they could be superposed and interpreted as 1 and 0 with certain probabilities, which is the characteristic trait of quantum bits. And combining many of them in logic gates and more complex structures they could eventually become a quantum computer.

Since these qubits would have topological protection they would be orders of magnitude safer than the actual ones and also more efficient, because it would not be necessary to have tens or hundreds of redundant physical qubits in order to have a logical one able to store 1 or 0. As we said a few pages earlier, this would be a major breakthrough in quantum computing and would enable us to solve problems much more complex than the ones being done by the most powerful supercomputers.




# 4.Practical Component: Bernevig-Hughes-Zhang Model in HgTe Quantum Wells and the Manifestation of the Topological Insulating State.

## 4.1. Introduction to the Practical Component

In this practical section, we aim to verify how band structures manifest in a prototypical topological insulator mercury telluride (HgTe) and to visualize the current density within the material. To achieve this, we have synthesized various concepts explored within the field of topological insulators.

## 4.2. Theoretical Framework: The Effective BHZ Hamiltonian

To rigorously interpret the numerical simulation of the BHZ model, it is necessary to explicate the mathematical model it implements: the Bernevig-Hughes-Zhang Hamiltonian. This model is an effective low-energy theory derived via perturbation theory near the center of the Brillouin zone, k=0.

### 4.2.1 Derivation and Matrix Structure

The model describes the dynamics of four relevant bands near the Fermi energy (E ≈ 0): two electron bands |E1,±⟩ (derived from s-orbitals , $\Gamma_6$) and two heavy hole bands |H1,±⟩ (derived from p-orbitals, $\Gamma_8$), where ± indicates the spin projection (or more precisely, the total angular momentum $m_j$). Due to time-reversal symmetry and spatial inversion symmetry (in the axial symmetry approximation), the full 4x4 Hamiltonian decouples into two independent 2x2, one for each spin sector.

The Hamiltonian takes the block-diagonal form:

$$H_{BHZ}(\mathbf{k}) = \begin{pmatrix} H(\mathbf{k}) & 0 \\ 0 & H^*(-\mathbf{k}) \end{pmatrix}$$

The upper and lower blocks are related by time-reversal symmetry. H(k), which describes the "spin-up" states, is expressed in the basis |E1,+⟩ ,|H1,+⟩ as:

$$H(\mathbf{k}) = \epsilon(\mathbf{k})\mathbb{I} + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma} = \begin{pmatrix} \epsilon(\mathbf{k}) + M(\mathbf{k}) & A(k_x - ik_y) \\ A(k_x + ik_y) & \epsilon(\mathbf{k}) - M(\mathbf{k}) \end{pmatrix}$$

Where, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices acting on the orbital subspace (E1, H1)

1. **Mass Term, M(k):**

$$M(\mathbf{k}) = M - B(k_x^2 + k_y^2)$$

This term describes the energy gap (band gap) at k=0 and its evolution with momentum. If M·B > 0, the band ordering is conventional (Normal Insulator). If M·B< 0, the bands are inverted (Topological Insulator). The quadratic term $Bk^2$ is necessary for the regularization of the model, ensuring that band inversion is localized at the center of the Brillouin zone.

2. **Hybridization Term,** $A(k_x \pm ik_y)$**:**

This off-diagonal term couples the E1 and H1 bands. It is linear in momentum k, analogous to the kinetic term in the Dirac equation. The parameter A represents the effective Fermi velocity of the edge states ($v_f = A/\hbar$). It is responsible for preventing band crossing in the bulk away from k=0.

3. **Particle-Hole Symmetry Breaking Term**, $\epsilon(k)$:

$$\epsilon(\mathbf{k}) = C - D(k_x^2 + k_y^2)$$

This term adds a global curvature to all bands, breaking the symmetry between

the conduction and valence bands. Although quantitatively adjusting the model to real experiments is necessary, it does not affect the system's topology provided the gap remains open. While often neglected (C=D=0) in simplified theoretical discussions to highlight chiral symmetry, its effect is visible in the asymmetry of the bulk bands in realistic simulations such as ours.

### 4.2.2 Material Parameters in the Simulation

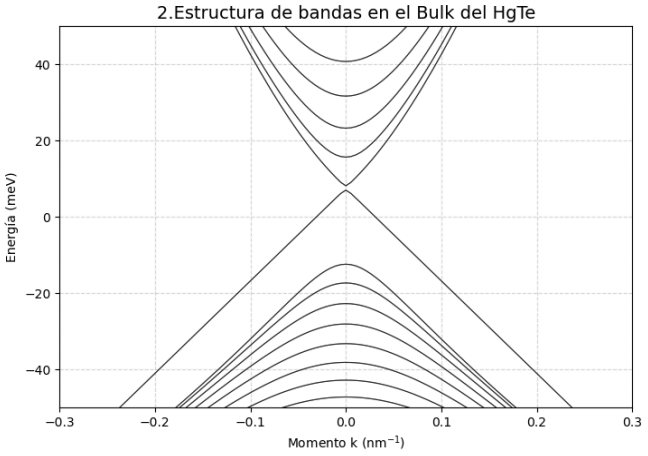
The validity of the visual results depends on the numerical parameters introduced into the code. Based on standard literature, the values for a 7.0 nm HgTe quantum well (topological regime) are approximately:

- **A (Fermi Velocity) ≈**3.65 eV·Å.
- **B (Newtonian Mass) ≈** -68.6 eV·Å^2.
- **D (Asymmetry) ≈** -51.2 eV·Å^2.
- **M (Topological Gap) ≈** -10 meV.

These values define the axis scales in the resulting images and confirm that the simulation operates within the band inversion regime.

## 4.3. Interpretation of Results

### 4.3.1. Bulk Band Structure

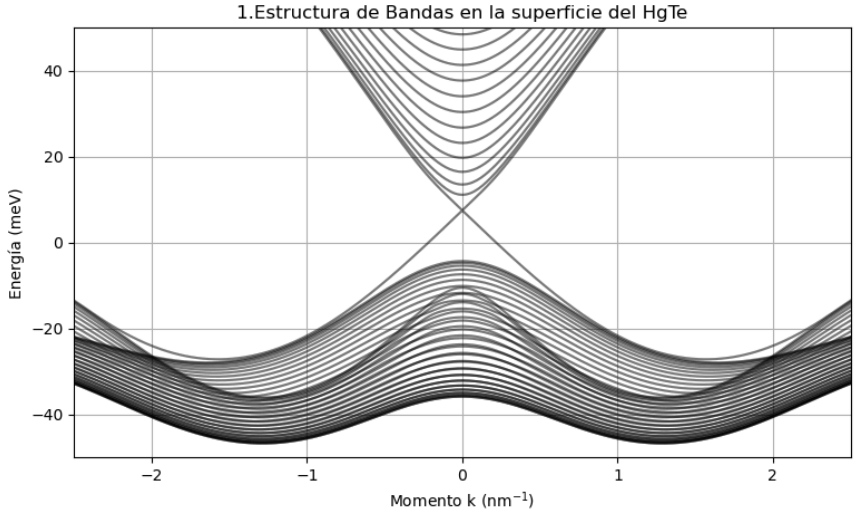



The image displays the energy dispersion versus momentum k. Two main bands are clearly observed, separated by an energy gap of approximately 20 meV (from -10 to +10 meV). Also we can observe:

**Mass Gap (2|M|):** The minimum separation at k=0 corresponds to the 2M term of the Hamiltonian. The existence of this gap confirms that the bulk of the material is insulating; there are no states available for electron conduction with energies near zero.

**Symmetry:** The symmetry E(k) = E(-k) is a consequence of the time-reversal and spatial inversion symmetries present in the simplified model.

## 4.3.2. Surface Band Structure

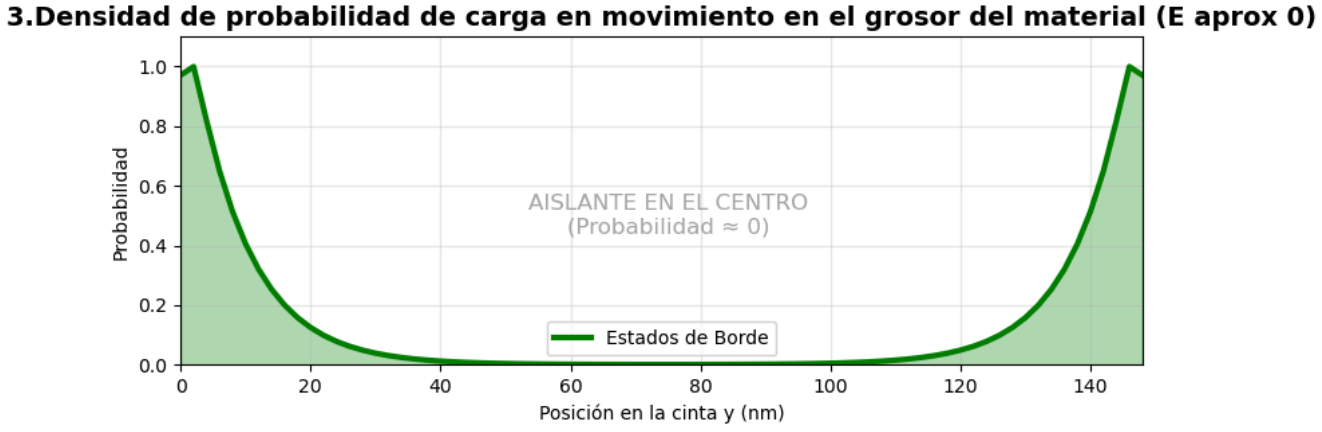



This graph shows the energy spectrum for the ribbon geometry. Unlike the bulk plot, we find "X"-shaped crossing lines within the forbidden bulk gap; two lines cross linearly from the valence band to the conduction band, intersecting at k=0.

**Dirac Dispersion:** The linearity of the crossing bands ($E \propto \hbar v_f k$) indicates that charge carriers at the edges behave as massless Dirac fermions. The slope of these lines is directly determined by the parameter A of the Hamiltonian.

**Topological Protection:** The crossing at k=0 is a degeneracy point protected by time-reversal symmetry. According to Kramer's theorem, in a fermionic system with TRS, states at invariant momenta (such as k=0) must be at least doubly degenerate. Far from k=0, spin-orbit coupling breaks this degeneracy. If the system were trivial, the bands could open a gap and separate; in the topological state ($Z_2$=1), this does not occur, ensuring conductivity.

## 4.3.3. Probability Density (Wavefunction)



The graph shows the probability of finding the electron $(\rho(y))$ across the width of the ribbon. The function presents maximum peaks at the edges (y=0 and y=L) and decays rapidly toward zero in the center.

**Spatial Localization:** This image is the real-space confirmation that the states crossing the gap in Image 1 are, effectively, edge states. They are not distributed uniformly throughout the material (as metallic states of an ordinary conductor would be), but rather confined to the boundaries.

**Insulating Center:** The null density in the central region (y = 75 nm) demonstrates the insulating character of the bulk. An electron injected into an edge state will travel along the wall without penetrating the volume.

**Decay Length ($\varepsilon$):** The drop in probability follows an exponential law $|\psi(y)|^2 \propto e^{\frac{-2y}{\varepsilon}}$. Theoretically, this penetration length is given by the ratio between hybridization and mass: $\varepsilon \approx |A/M|$

Observation: If the magnitude of the gap M were reduced in the simulation (approaching the phase transition $d \approx d_c$), the length $\varepsilon$ would increase, the edge states would broaden, and eventually merge in the center, destroying the topological protection. The clear separation in Image 3 indicates that the width of the simulated ribbon is sufficient to behave as an ideal topological system.

# 5.Conclusions

As seen, topological behaviors can appear in a wide variety of materials and experiments, in some cases just as a curiosity but in others with the possibility to completely revolutionize entire fields of physics. And it is precisely this potential which makes it so important to continue investigating it, in comparison with other branches of physics this one is extremely recent and particular. Not only does it manage to explain the characteristics of exotic materials with great precision, but it does so by taking a mathematical field, completely abstract and thought to be “useless” in the real world and turning it into a key fundamental of modern condensed matter physics.

In addition we are glad to have employed real life investigation techniques such as computer simulation or scientific papers analysis. From our perspective this project has broaden our minds and allowed us to discover a fascinating field with much work left to do.

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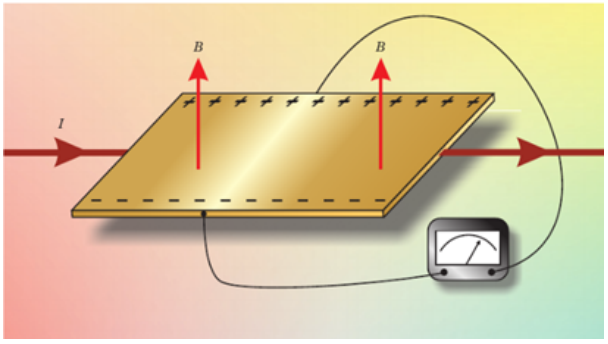
# Appendix A: Classical Hall Effect

To begin this section, it is essential that we understand what the Hall effect is in classical physics. In 1879, James Clerk Maxwell consolidated his equations, where, among many other assertions, he maintained that the magnetic force acted on the physical conductor transporting the current, and not directly on the electric current itself. Edwin Hall disagreed with this and decided to prove it in an experiment.

Using a thin gold leaf (to maximize current density and confine the flow to a quasi-two-dimensional plane) and the most sensitive batteries and galvanometers of the time, Hall managed to measure a tiny but undeniable transverse voltage when applying a magnetic field perpendicular to the current. This voltage, $V_H$ , demonstrated unequivocally that the charge carriers were deflected by the magnetic field and not the conductor, as Maxwell argued.




Now, to explain the quantum Hall effect, we must introduce a mathematical-physical relationship that will later be very useful to understand the differences between the classical and quantum effects. From the experiment, Hall derived a relationship he called the Hall Coefficient ($R_H$) ; this is the constant of proportionality between the transverse field and the product of the current and the magnetic field. $R_H = \frac{E_H}{J_x B}$

And we can define the Hall Resistivity as: $\rho_{xy} = \frac{E_H}{J_x B}$

In the classical regime, the Hall resistivity is strictly linear with the magnetic field. A graph of this is a straight line passing through the origin, with a slope determined inversely by the electron density.

# Appendix B: Computational Analysis

The core of this section lies in explaining the code that is capable of transforming the abstract equations above into graphical representations where the expected results can be observed. Since computers cannot handle infinite continuous spaces, this simulation necessarily employs discretization methods.

## B.1. Hamiltonian Discretization with Finite Differences

The first logical step in the code is to convert the continuous Hamiltonian H(k) into a lattice matrix (lattice Hamiltonian). This is achieved via Peierls substitution or finite difference discretization on a square lattice with lattice constant a.

Continuous derivatives are replaced by differences:

$$k_i \to -i\partial_i \implies \partial_x \psi(x) \approx \frac{\psi(x+a) - \psi(x-a)}{2a}$$

$$k_i^2 \to -\partial_i^2 \implies \partial_x^2 \psi(x) \approx \frac{\psi(x+a) - 2\psi(x) + \psi(x-a)}{a^2}$$

Applying this transformation to the BHZ model terms:

**Mass Term and Kinetic Energy ($k^2$):**

Terms proportional to $k^2$ (parameters B and D) generate couplings between neighboring sites and local terms.

$$M - Bk^2 \longrightarrow \left(M - \frac{4B}{a^2}\right)\mathbb{I} + \frac{B}{a^2}\sum_{\delta} e^{i\mathbf{k}\cdot\boldsymbol{\delta}}$$

In the lattice representation, this means each site has a self-energy modified by B and connects to its nearest neighbors with a hopping strength proportional to $B/a^2$.

**Linear Term (k):**

The term $A(k_x\sigma_x \pm ik_y\sigma_y)$ generates asymmetric and imaginary hops.

$$Ak_x\sigma_x \longrightarrow \frac{A}{2ia}(\hat{c}_{i+x}^{\dagger}\sigma_x\hat{c}_i - \hat{c}_i^{\dagger}\sigma_x\hat{c}_{i+x})$$

This discretization process is used to avoid the "fermion doubling" problem. The quadratic term ($Bk^2$) acts as a regulator, assigning a very large mass to states at the edges of the Brillouin zone ($k = \frac{\pi}{a}$), ensuring that the low-energy physics observed in the images corresponds solely to the Γ point, faithful to the continuous model.

## B.2. Basis for Band Structure Calculations

### Basis for Bulk Band Structure (Image 2)

To generate Image 2, the code assumes Periodic Boundary Conditions (PBC) in both the x and y directions. The system is effectively an infinite torus.

- The code defines a grid of points in k-space (Brillouin Zone), typically from -π to +π .

- For each pair ($k_x$, $k_y$), the code constructs the numerical 4x4 matrix of the Hamiltonian $H_{BHZ}(k)$ using parameters A, B, C, D, M.
- This small matrix is diagonalized using standard linear algebra code (numpy.linalg.eigh in Python), returning 4 energy eigenvalues $E_n(k)$.
- These eigenvalues are plotted against k. The 4 bands visually appear as 2 degenerate parabolas (conduction and valence).

## Basis for Surface Band Structure (Image 1)

This is the most computationally complex part. To simulate the surface (ribbon) and observe edge states, the code breaks periodicity in one direction (say y) while maintaining it in the other (x).

**Geometry:** A strip of finite width W is defined, discretized into $N_y$ sites in the y-direction.

**Hilbert Space Basis:** The size of the Hamiltonian matrix now scales with the width of the strip. The dimension is $4N_y$ x $4N_y$.

**Matrix Construction:** The code iterates over values of the conserved momentum $k_x$ .Where diagonal blocks represent the energy within each 1D chain in x (including terms dependent on $k_x$), while off-diagonal blocks couple chain $n_y$ with $n_y$+1 and $n_y$ -1. Finally, "hard-wall" boundary conditions are applied at y=0 and y=W (simply by not including hoppings outward from the matrix).

**Diagonalization:** The $4N_y$ x $4N_y$ is diagonalized.

**Result:** $4N_y$ eigenvalues are obtained for each $k_x$. Plotting them all yields the "spaghetti" structure of Image 1, showing the projected bulk bands and the states crossing the gap.

## Calculation of Probability Density (Image 3)

Once the ribbon Hamiltonian is diagonalized for a specific $k_x$, the code extracts the eigenvalues.Let $\psi_n$ be the eigenvector corresponding to an energy state $E_n$ found within the gap (an edge state) having $4N_y$ components ( $\psi_n = [\phi_{1,E\uparrow}, \phi_{1,H\uparrow}, \ldots\ldots, \phi_{N_y,H\downarrow}]$ ). The code calculates the local probability density at each site $y_i$ by summing the moduli of the components and the spin at that site:

$$\rho(y_i) = \sum_{\alpha \in \{E\uparrow, H\uparrow, E\downarrow, H\downarrow\}} |\Psi_{n,\alpha}(y_i)|^2$$

# Appendix C: Code

## C.1 Surface Band Simulation (Image 1)

```
""" Script: sim_surface_bands.py Descripción:
Calcula la estructura de bandas de una nanocinta de HgTe.
Modelo: Hamiltoniano BHZ (Bernevig-Hughes-Zhang).
"""


import kwant
import numpy as np
import matplotlib.pyplot as plt
import warnings

# Ignorar advertencias para limpieza
warnings.filterwarnings("ignore")

# Definición del Hamiltoniano BHZ (4x4)
hamiltonian_bhz = """
 (C + M - B * (k_x**2 + k_y**2)) * kron(sigma_0, sigma_z)
 - D * (k_x**2 + k_y**2) * kron(sigma_0, sigma_0)
 + A * k_x * kron(sigma_z, sigma_x)
 - A * k_y * kron(sigma_0, sigma_y)
"""

a=7 # 'nm'
def make_system(L=400, W=300, a=a):
    """
    Construye un sistema de dispersión (scattering region) y sus leads.
    """
    # Parámetros (Aseguramos que sean floats) Parámetros verificados (König et al. 2008,7nm HgTe QW)

    params = dict(A=364.5, B=-686.0, D=-512.0, M=-10.0, C=0.0)

    # 1. Discretización automática
    template = kwant.continuum.discretize(hamiltonian_bhz, grid=a)

    # 2. Definición de la red y el constructor
    lat = kwant.lattice.square(a)
    syst = kwant.Builder()

    # 3. Relleno de la región de dispersión
    def shape(site):
        (x, y) = site.pos
        return 0 <= x < L and 0 <= y < W

    syst.fill(template, shape, (0, 0))

    # 4. Leads (Contactos semi-infinitos)
    sym_left = kwant.TranslationalSymmetry((-a, 0))
    lead = kwant.Builder(sym_left)


    def lead_shape(site):
        (x, y) = site.pos
        return 0 <= y < W
```

```
    lead.fill(template, lead_shape, (0, 0))

    syst.attach_lead(lead)
    syst.attach_lead(lead.reversed())

    return syst.finalized(), params

def plot_bandstructure(syst, params):
    # Usamos el lead 0 (izquierdo) porque “son lo mismo” (el derecho y el izquierdo)
    lead = syst.leads[0]

    bands = kwant.physics.Bands(lead, params=params)
    momenta = np.linspace(-np.pi, np.pi, 500)
    energies = [bands(k) for k in momenta]

    plt.figure(figsize=(9, 5))
    plt.plot(momenta, energies, 'k-', alpha=0.3)
    plt.xlabel(r"Momento k (nm$^{-1}$)")
    plt.ylabel("Energía (meV)")
    plt.title("1.Estructura de Bandas en la superficie del HgTe")
    plt.ylim(-50, 50)
    plt.xlim(-2.5,2.5)
    plt.grid(True)
    plt.show()


if __name__ == "__main__":
    sistema_finalizado, parametros = make_system()
    plot_bandstructure(sistema_finalizado, parametros)
```

## C.2 Bulk Band Simulation (Image 2)

```
"""
Script: sim_bulk_bands.py
Descripción: Simulación de bandas de volumen (Bulk) mediante diferencias finitas manuales.
(Originalmente lo hubiera hecho otra vez con kwant pero por alguna razón no funcionaba
correctamente)
"""

import numpy as np
import matplotlib.pyplot as plt
import warnings

warnings.filterwarnings("ignore")


# 1. Configuración y parámetros
# Parámetros del material (HgTe 7.0 nm - König et al. 2008)
A = 364.5      # meV nm
B = -686.0     # meV nm^2
D = -512.0     # meV nm^2
M = -10.0      # meV (Masa negativa indica régimen topológico)
C = 0.0        # meV

# Parámetros de la simulación (Geometría de Cinta)
W = 150.0      # Anchura de la cinta en nm
```

```
a = 2.0        # Constante de red (nm)
Ny = int(W / a) # Número de sitios en la red (dirección y)


# Matrices de Pauli
s0 = np.eye(2)
sx = np.array([[0, 1], [1, 0]], dtype=complex)
sy = np.array([[0, -1j], [1j, 0]], dtype=complex)
sz = np.array([[1, 0], [0, -1]], dtype=complex)


# 2. Construcción del hamiltoniano
def make_hamiltonian(kx):
    """
    Construye la matriz Hamiltoniana de Tight-Binding (4Ny x 4Ny)
    para un momento kx dado.
    """
    # Términos diagonales (On-site)
    # E(k) = C - D(kx^2 + ky^2) -> ky^2 se convierte en 2/a^2 en diferencias finitas
    # M(k) = M - B(kx^2 + ky^2)
    eps_k = C - D * (kx**2 + 2/a**2)
    m_k   = M - B * (kx**2 + 2/a**2)

    # Bloques 2x2 para cada espín
    # Bloques de espín
    h_up = (eps_k * s0) + (m_k * sz) + (A * kx * sx)
    h_dn = (eps_k * s0) + (m_k * sz) - (A * kx * sx)

    # Ensamblaje del bloque on-site 4x4
    H_onsite = np.zeros((4, 4), dtype=complex)
    H_onsite[0:2, 0:2] = h_up
    H_onsite[2:4, 2:4] = h_dn

    # Términos de Hopping (Salto vertical)
    # Ty = (D + B*sz)/a^2 - i*A/(2a)*sy
    # Para spin down, usamos el conjugado de sy (sy* = -sy), pero el término A es A*ky*sy
    # ky -> -i d/dy. La discretización correcta lleva a:

    ty_up = (D * s0 + B * sz) / a**2 - 1j * A / (2*a) * sy
    ty_dn = (D * s0 + B * sz) / a**2 + 1j * A / (2*a) * sy # Nota: cambio de signo

    T_y = np.zeros((4, 4), dtype=complex)
    T_y[0:2, 0:2] = ty_up
    T_y[2:4, 2:4] = ty_dn

    # Matriz dispersa llena (Densa para simplicidad académica)
    size = 4 * Ny
    H_tot = np.zeros((size, size), dtype=complex)

    for i in range(Ny):
        # Diagonal
        H_tot[4*i : 4*(i+1), 4*i : 4*(i+1)] = H_onsite

        if i < Ny - 1:
            # Hopping derecha (i -> i+1)
            H_tot[4*i : 4*(i+1), 4*(i+1) : 4*(i+2)] = T_y
            # Hopping izquierda (i+1 -> i)
```

```
            H_tot[4*(i+1) : 4*(i+2), 4*i : 4*(i+1)] = T_y.conj().T

    return H_tot


# 3. Cálculo
def main():
    k_vals = np.linspace(-0.4, 0.4, 151)

    # Inicialización correcta de listas
    all_eigenvalues = []

    for k in k_vals:
        H = make_hamiltonian(k)
        # Diagonalización
        evals, evecs = np.linalg.eigh(H)

        all_eigenvalues.append(evals)

    # Convertir a arrays numpy para facilitar el indexado
    all_eigenvalues = np.array(all_eigenvalues) # (Nk, 4Ny)


    # 4. Graficación
    fig = plt.figure(figsize=(18, 12))
    ax1 = fig.add_subplot(2, 2, 1)
    ax1.set_title("2.Estructura de bandas en el Bulk del HgTe", fontsize=14)
    ax1.set_ylabel("Energía (meV)")
    ax1.set_xlabel(r"Momento k (nm$^{-1}$)")

    # Graficamos todas las bandas en negro sólido para ver la cuantización
      for i in range(4*Ny):
        ax1.plot(k_vals, all_eigenvalues[:, i], c='k', lw=0.8, alpha=0.6)

    ax1.set_ylim(-50, 50)
    ax1.set_xlim(-0.3,0.3)
    ax1.grid(True, linestyle='--', alpha=0.5)

# Bloque de ejecución principal
if __name__ == "__main__":
    main()
```

## C.3 Code for simulating the probability density of charge in motion throw the material (Image 3)

```
"""
Script: sim_density_profile.py
Descripción: Calcula la densidad de probabilidad espacial de los estados de energía cero.
"""

import kwant
import numpy as np
import sympy
import matplotlib.pyplot as plt
import warnings
warnings.filterwarnings("ignore")
```

```
# 1. Construcción del sistema
def make_system(W=150, a=2.0):
    """
    Construye el sistema con corrección de bordes para evitar errores de índice.
    """
    # 1. Definimos símbolos NO CONMUTATIVOS para operadores
    k_x, k_y = sympy.symbols('k_x k_y', commutative=False)
    A, B, C, D, M = sympy.symbols("A B C D M")

    # 2. Matrices de Pauli como objetos SymPy
    sigma_0 = sympy.eye(2)
    sigma_x = sympy.Matrix([[0, 1], [1, 0]])
    sigma_y = sympy.Matrix([[0, -1j], [1j, 0]])
    sigma_z = sympy.Matrix([[1, 0], [0, -1]])

    # 3. Construimos el Hamiltoniano (Modelo BHZ)
    k_sq = k_x**2 + k_y**2
    eps_k = C - D * k_sq
    m_k   = M - B * k_sq

    # Bloques de espín
    h_up = eps_k * sigma_0 + m_k * sigma_z + A * k_x * sigma_x - A * k_y * sigma_y
    h_dn = eps_k * sigma_0 + m_k * sigma_z - A * k_x * sigma_x - A * k_y * sigma_y

    # Matriz 4x4 completa
    hamiltonian_4x4 = sympy.diag(h_up, h_dn)

    # 4. Discretización
    template = kwant.continuum.discretize(hamiltonian_4x4, coords="xy", grid=a)

    # 5. Construcción del Sistema
    sym = kwant.TranslationalSymmetry((a, 0))
    syst = kwant.Builder(sym)


    # Usamos una pequeña tolerancia (epsilon) para evitar que, por error de redondeo,
    # se incluya un sitio extra justo en el borde W.
    def shape(site):
        (x, y) = site.pos
        # Aseguramos que y sea estrictamente menor que W con margen de seguridad
        return 0 <= y < (W - 1e-6)

    syst.fill(template, shape, (0, 0))

    # Parámetros numéricos
    params = dict(A=364.5, B=-686.0, D=-512.0, M=-30.0, C=0.0) # König et al. 2008

    return syst.finalized(), params


# 2. Cálculo
def main():
    W = 150.0
    a = 2.0
    k_range = 0.15
```

```
syst, params = make_system(W, a)

# Extracción de matrices
h_cell = syst.cell_hamiltonian(params=params)
h_hop = syst.inter_cell_hopping(params=params)

# Validamos las dimensiones
# Calculamos cuántos sitios reales hay en la matriz Hamiltoniana
# Cada sitio tiene 4 orbitales.
Ny_hamiltonian = h_cell.shape[0] // 4

# Obtenemos los sitios del sistema
sites = syst.sites
y_positions = np.array([s.pos[1] for s in sites])

# Si hay discrepancia, recortamos para que coincidan
if len(y_positions) != Ny_hamiltonian:
    # Tomamos solo los primeros N sitios que coinciden con la matriz
    y_positions = y_positions[:Ny_hamiltonian]

# Ordenamos espacialmente
sort_idx = np.argsort(y_positions)
y_sorted = y_positions[sort_idx]
Ny = len(y_sorted)

k_vals = np.linspace(-k_range, k_range, 201)
evals_list = []
color_list = []

vecs_k0 = None
energies_k0 = None
idx_k0 = np.argmin(np.abs(k_vals))

for i, k_real in enumerate(k_vals):
    k_adim = k_real * a

    # H(k) manual
    phase = np.exp(-1j * k_adim)
    h_k = h_cell + h_hop * phase + h_hop.conj().T * phase.conj()

    # Diagonalización
    vals, vecs = np.linalg.eigh(h_k)
    evals_list.append(vals)

    if i == idx_k0:
        energies_k0 = vals
        vecs_k0 = vecs


    edge_weight = []
    limit_idx = int(Ny * 0.15)

    for band in range(len(vals)):
        psi = vecs[:, band]

        # Reshape seguro usando el Ny validado
        psi_site = psi.reshape(Ny, 4)
```

```
            psi_sorted = psi_site[sort_idx] # Ahora esto no puede fallar

            prob = np.sum(np.abs(psi_sorted)**2, axis=1)
            w_edge = np.sum(prob[:limit_idx]) + np.sum(prob[-limit_idx:])
            edge_weight.append(w_edge)

        color_list.append(edge_weight)


    # 3. Graficamos
    fig = plt.figure(figsize=(8, 6))
    ax3 = fig.add_subplot(2, 1, 2)

    idx_sorted_en = np.argsort(np.abs(energies_k0))
    idx_edge_states = idx_sorted_en[:2]

    psi_edge_sum = np.zeros(Ny)
    for idx in idx_edge_states:
        vec = vecs_k0[:, idx].reshape(Ny, 4)
        vec_sorted = vec[sort_idx]
        psi_edge_sum += np.sum(np.abs(vec_sorted)**2, axis=1)

    psi_edge_sum /= np.max(psi_edge_sum)

    ax3.set_title("3.Densidad de probabilidad de carga en movimiento en el grosor del
material (E aprox 0)", fontsize=14, fontweight='bold')
    ax3.plot(y_sorted, psi_edge_sum, color='green', lw=3, label='Estados de Borde')
    ax3.fill_between(y_sorted, psi_edge_sum, color='green', alpha=0.3)

    ax3.set_xlabel("Posición en la cinta y (nm)")
    ax3.set_ylabel("Probabilidad")
    ax3.set_xlim(2, W-4)
    ax3.set_ylim(0, 1.1)

    ax3.text(W/2, 0.5, "AISLANTE EN EL CENTRO\n(Probabilidad ≈ 0)",
             ha='center', va='center', fontsize=12, color='gray', alpha=0.7)

    ax3.grid(True, alpha=0.3)
    ax3.legend()

    plt.tight_layout()
    plt.show()

if __name__ == "__main__":
    main()
```