



Topological Quantum Matter

Nobel Lecture, December 8, 2016

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ABSTRACT

Nobel Lecture, presented December 8, 2016, Aula Magna, Stockholm University. I will describe the history and background of three discoveries cited in this Nobel Prize: The “TKNN” topological formula for the integer quantum Hall effect found by David Thouless and collaborators, the Chern Insulator or quantum anomalous Hall effect, and its role in the later discovery of time-reversal-invariant topological insulators, and the unexpected topological spin-liquid state of the spin-1 quantum antiferromagnetic chain, which provided an initial example of topological quantum matter. I will summarize how these early beginnings have led to the exciting, and currently extremely active, field of “topological matter.”

What we now know as “Topological quantum states” of condensed matter were first encountered around 1980, with the experimental discovery of the integer (Klitzing *et al.*, 1980), and later fractional (Tsui *et al.*, 1982) quantum Hall effects in the two-dimensional electron systems in semiconductor devices, and the theoretical discovery of the entangled gapped quantum spin-liquid state of integer-spin “quantum spin chains” (Haldane, 1981a, 1983a,b), which was later experimentally confirmed (Buyers *et al.*, 1986) in crystals of the organic chain molecule NENP. The common feature of these discoveries was their unexpectedness and the surprise that they engendered: they did not fit into the then-established paradigms of “condensed matter physics” (previously known as “solid

state physics”). It was not at the time apparent that there could be any connection between these two surprises, but now, especially following the classification work of Xiao-Gang Wen (Chen *et al.*, 2013), we understand that their common feature is that they involve “topologically non-trivial” entangled states of matter that are fundamentally different from the previously-known “topologically trivial” states, and this lies at the heart of their unexpected properties.

Topology is the branch of mathematics originally used to classify the shapes of three-dimensional objects such as soccer balls, rugby (or American football) balls and coffee mugs (without a handle), which are “topologically trivial” surfaces without holes, and bagels, doughnuts, pretzels, and coffee cups with a handle, which are “non-trivial surfaces” with one or more holes. An ant crawling on such a “non-trivial” surface could walk around a closed path (one that ends at the same point that it started) that cannot be smoothly shrunk to a tiny circle around a point on the surface. These original ideas of topology were greatly generalized and made abstract by mathematicians, but the central idea, that things are only “topologically equivalent” if they can smoothly be transformed into each other, remains as its key idea. The essential feature is that different topologies are classified by whole numbers, like the number of holes in a surface, which cannot change gradually.

Entanglement is a central property of quantum mechanics whereby, if the state of a system is described in terms of the quantum state of its parts (typically if it is spatially separated into two halves), a measurement of a property localized in one of the two halves affects the state of the other half of the system. The “topology” of the “topological states of matter” celebrated in this Nobel Prize is more abstract than that of the shapes of everyday objects such as soccer balls and coffee cups, but distinguishes different types of “quantum entanglement” that cannot smoothly be transformed into one another, perhaps while some protective symmetries are being respected. In this case, a quantum state has “topologically trivial” entanglement if it can be smoothly transformed to a state where each part of the system is in an independent state where a measurement on that part has no effect on other parts of the system (this is called a “product state”). In the case of quantum spin systems (descriptions of non-metallic magnets), it turned out that almost all previously theoretically-described states were “topologically trivial,” so there was no precedent for the surprising properties of a non-trivial “topological state.”

It took some time for the general understanding that there was a large class of new “topological states of matter” to emerge. An early milestone was the discovery (Thouless *et al.*, 1982) by David Thouless, and collaborators Mahito Kohmoto, Marcel den Nijs and Peter Nightingale (TKNN) of a remarkable

formula that was soon recognized by the mathematical physicist Barry Simon (Simon, 1983) as just being the “first Chern class invariant” from the abstract mathematical topology of so-called “ $U(1)$ fiber bundles,” with an essential connection to a contemporaneous development, the “adiabatic quantum phase” discovered in 1983 by Michael Berry (Berry, 1984). As I am also presenting part of David Thouless’ Nobel-Prize-winning work, I will describe this first in my lecture, and begin with the quantum Hall effect, for which two Nobel Prizes (1985 and 1998) have already been awarded.

In the presence of a uniform magnetic field with flux density B , charge- e electrons bound to a two-dimensional surface through which the magnetic field passes move in circular “Landau orbits.” According to quantum mechanics, this periodic motion gives rise to a discrete set of positive energy levels of the electrons called “Landau levels.” In the simplest model for these Landau levels, the period $T = 2\pi/\omega_c$ of the circular motion is independent of the radius of the circular motion, and the allowed energies of the Landau levels are those of a harmonic oscillator, $(n + \frac{1}{2})\hbar\omega_c$, where $\omega_c = eB/m_e$ is the so-called “cyclotron frequency.” Assuming that the surface has translational symmetry, so all points on the surface are equivalent, the energy of each state in a Landau level is independent of the position of the center of the orbit, and the Landau level is highly (macroscopically) degenerate. The number of independent one-particle states in the Landau level is proportional to the area A of the system, in fact there are BA/Φ_0 states in each Landau level, where $\Phi_0 = h/e$ is the (London) quantum of magnetic flux.

The Pauli principle says that not more than one electron can “occupy” any independent one-particle state, and the Landau levels are somewhat analogous to the levels (1s, 2p, 3d . . .) of the simple quantum mechanical model of the atom, familiar from high-school chemistry. However, instead of these levels accommodating finite and fixed numbers (2, 6, 10 . . .) of states available to be “filled,” the number of states in a Landau level is huge (perhaps of order 10^{12} in a real sample) and varies with the magnetic field. Since the number of mobile electrons of the 2D surface is essentially fixed, it could in principle be possible to get things “just right” by “fine-tuning” the magnetic field so that in the ground state of the system, one or more Landau levels are completely filled, and the rest are completely empty, so that an energy gap separates the energy of the “highest occupied state” (the “HOMO” in quantum chemistry) and the “lowest unoccupied state” (or “LUMO”), making the system analogous to an intrinsic (undoped) semiconductor. Under these artificial “toy model” conditions, a simple calculation of the Hall conductivity σ^{xy} of the system would indeed reproduce the quantum Hall effect with the universal value $\sigma^{xy} = ne^2/h$ (that depends only on

material-independent fundamental constants and a whole number n , which is the number of occupied Landau levels), that would correspond to the results measured by von Klitzing.

The flaw in this naïve explanation of the integer QHE is that it requires exquisite fine-tuning of the strength of the magnetic field. In contrast, it was the *insensitivity* to the fine-tuning of the magnetic field strength that alerted von Klitzing to the effect. He “switched on” the field to apply it to a device through which a fixed current was flowing stabilized by a constant current source, and observed that when things stabilized, a digital voltmeter always showed the same Hall voltage across the sample to many significant figures. (The story is told that he first thought the voltmeter was broken!) Of course, each time the magnetic field was “turned on” was different, so the final field would never have been the same on each run of the experiment, and certainly would never have “accidentally” taken the precise “magic value” of the naïve explanation. It is fortunate that von Klitzing switched on the magnetic field with a fixed current through the sample, rather than switched on the current at fixed field, as the coincidence of the unchanged digital voltmeter readings would then never have happened!

The real samples, though comparatively clean, do not have the translational invariance that makes each state in a given Landau level have exactly the same energy. A local electric potential at the center of a given circular Landau orbit varies randomly from point to point, sometimes raising and sometimes lowering the energy, “broadening” the Landau level. The initial attempts to explain the effect focused on this effect of disorder, and found that, while two-dimensional electron systems with disorder generally have “localized” states, this is modified in a magnetic field. In this case, the centers of the Landau orbits slowly precess (in opposite senses) around either local minima or local maxima of the potential, corresponding to localized states, but there is an energy at the center of the broadened Landau level at which the centers of the orbits move along open snakelike paths, and the states at that energy are “extended” as opposed to “localized.” In this picture, there is no gap between the “HOMO” and the “LUMO” which have equal energies (now called the “Fermi energy”), and, as the magnetic field strength is changed, the Fermi energy moves to keep the number of occupied states constant, but the integer n measured by von Klitzing only changes when the Fermi energy goes through the special energy at which extended states exist. This provided an explanation in terms of the somewhat arcane theory of localization that at first sight is not obviously topological, but what is now obvious as a very characteristically topological property emerged when Bert Halperin pointed out the importance of edge states (Halperin, 1982).

These edge states are easily seen as semiclassically as counterpropagating “skipping orbits” that precess around the boundary of the system in the opposite sense to that of the Landau orbits, when a particle in a Landau orbit intersects the boundary, and bounces off it (see Figure 1). Even without disorder in the interior of the disk, so that the energy gap between Landau levels remains, there is a continuous distribution of energy levels at the edge of the system that pins the Fermi level and accommodates the “spectral flow” of states between Landau levels as the field magnetic strength is changed, and removes the need for “fine tuning” of the magnetic field to have an energy gap in the interior of the sample. While the number of states in a Landau level changes with magnetic field strength, the number of states cannot change, so the states must flow between Landau levels: the gapless edge states provide the necessary “plumbing” connections between the Landau levels so states can be redistributed between them as the magnetic field changes.

The unavoidable edge states that transport particles in one direction only around the edge allow the robustness of the QHE to be understood in terms of the boundary of the system, but it is also valuable to understand it in terms of the bulk properties of the interior of the system. This is where the TKNN formula found by David Thouless and collaborators (Thouless *et al.*, 1982) enters the story. Thouless was inspired by the famous “Hofstadter butterfly” spectrum (Hofstadter, 1976) that results when there is a periodic potential on the 2D surface as well as magnetic flux (Figure 2). In this case, the energy band structure can be solved when the magnetic flux through the unit cell of the periodic

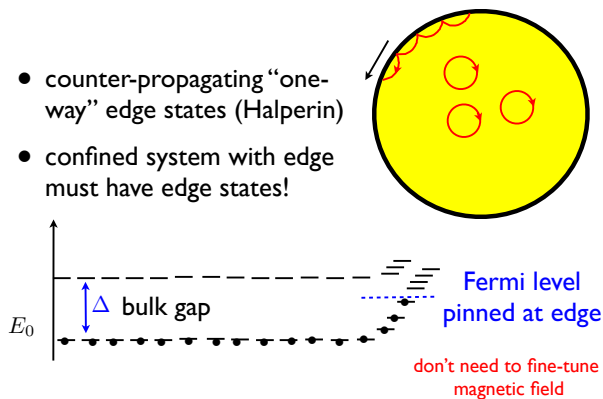


FIGURE 1. Simple energy-level picture for the integer quantum Hall effect, with an energy gap in the bulk stabilized by pinning of the Fermi level by gapless edge states. (The energy levels are shown as a function of radius in a disk-shaped sample).

potential is a rational number p/q , where p and q are relative prime numbers with no common factors. The solution depends very delicately on the precise values of p and q , as it must be solved in an enlarged “magnetic unit cell” through which the magnetic flux must be an integer in units of Φ_0 . The effect of the magnetic field is that each zero-field energy band that occurs in the absence of a magnetic field splits up into q energy bands, so that in going from a flux of $1/3$ per unit cell to $100/301$, what is one band at flux $1/3$ splits up into 100 much narrower bands even though the flux change is very small!

A very clear argument formulated by Robert Laughlin (Laughlin, 1981) had already shown that in the absence of electron-electron interactions, if the Fermi level is inside a gap of the bulk electronic spectrum, the Hall conductivity σ^{xy} in the low-temperature limit $T \rightarrow 0$ had to be an integer multiple of $e/\Phi_0 = e^2/2\pi\hbar$. In the bottom left-hand corner of the “Hofstadter butterfly,” where the magnetic flux through the unit cell is very small, the spectrum resembles that of simple Landau levels, with extremely narrow flat bands corresponding to a slightly widened Landau level, separated by large gaps. In this limit, the integer is just given by the number of filled Landau levels. But as the flux increases, the

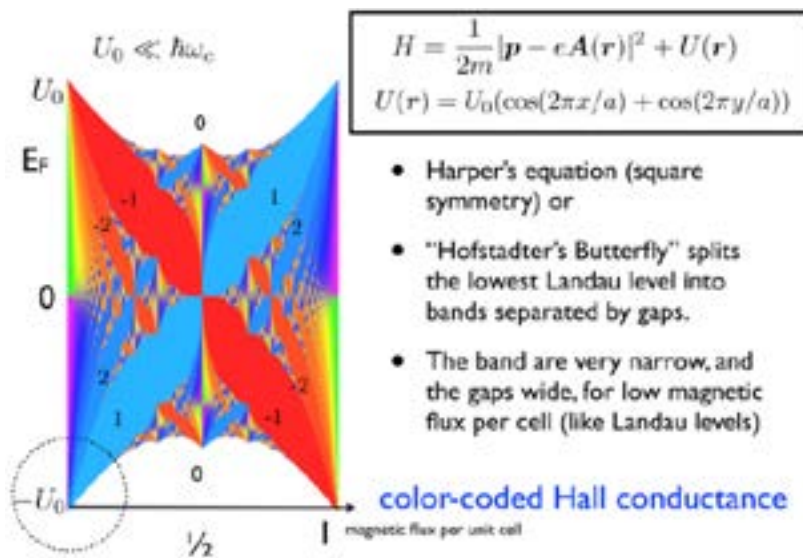


FIGURE 2. The “Hofstadter Butterfly” spectrum of electrons on a periodic lattice plus a uniform magnetic field, showing energy levels as a function of magnetic flux through a unit cell. The structure in the lower left corner becomes that of a system of simple Landau levels. Colors in gaps between subbands represent the different integer quantizations of the Hall effect if the Fermi level is in that gap. (Colored spectrum provided by D. Osadchy and J. Avron).

Landau levels split up into an intricate pattern of sub-bands which are separated by many more gaps, which open and close as the magnetic field changes. When the Fermi level is in one of these new gaps, the question posed by TKNN was, what is the integer that defines the low-temperature Hall conductivity?

Even though TKNN were working in the enlarged “magnetic unit cell,” the Bloch theorem remained valid, and showing the electronic wavefunctions had the form

$$\Psi_{k_n}(\mathbf{r}) = u_n(\mathbf{k}, \mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \quad (1)$$

where $u_n(\mathbf{k}, \mathbf{r})$ is a periodic function of \mathbf{r} defined in the magnetic unit cell (MUC). Here \mathbf{k} is a “Bloch vector” defined in the (magnetic) “Brillouin zone” (BZ) which in 2D is topologically equivalent to a torus, or doughnut shape. Using the fundamental Kubo formula for electrical conductivity, they found the formula

$$\sigma^{xy} = \frac{e^2}{2\pi\hbar} \sum_n \left(\frac{1}{2\pi} \int_{\text{BZ}} d^2\mathbf{k} F_n^{xy}(\mathbf{k}) \right)$$

$$F_n^{xy}(\mathbf{k}) = \frac{1}{2i} \int_{\text{MUC}} d^2\mathbf{r} \left(\frac{\partial u_n^*}{\partial k_x} \frac{\partial u_n}{\partial k_y} - \frac{\partial u_n^*}{\partial k_y} \frac{\partial u_n}{\partial k_x} \right)$$

Here n labeled the occupied electronic bands below the Fermi level. The remarkable property was that the integral of each periodic function $F_n^{xy}(\mathbf{k})$ over the magnetic Brillouin zone was 2π times an integer, in agreement with Laughlin’s result. TKNN realized that this had to be so, because $F_n^{xy}(\mathbf{k})$ could be written in the form

$$F_n^{xy}(\mathbf{k}) = \frac{\partial}{\partial k_x} A^y(\mathbf{k}) - \frac{\partial}{\partial k_y} A^x(\mathbf{k})$$

$$A_n^i = \frac{1}{2i} \int_{\text{MUC}} d^2\mathbf{r} \left(u_n^* \frac{\partial u_n}{\partial k_i} - u_n \frac{\partial u_n^*}{\partial k_i} \right)$$

leading to the key expression, as an integral around the Brillouin zone boundary (BZB) :

$$\sigma^{xy} = \frac{e^2}{2\pi\hbar} \sum_n \frac{1}{2\pi} \oint_{\text{BZB}} dk_i A_n^i(\mathbf{k}) \quad (2)$$

I learned from Marcel den Nijs and Peter Nightingale that their recollection is that the inclusion (in a single paragraph) of this remarkable explicit general

formula in the paper (rather than formulas very specific to the Hofstadter model, which were the main aim of the paper) emerged as an “afterthought” while writing the paper! Another quote from den Nijs is that it was “the genius of David Thouless to choose the periodic potential generalization [to broaden the Landau level] rather than the random one, that was the essential step.” This shows the power of choosing the right (and tractable) toy model for which a full and explicit calculation can be done. While there has been continuing interest to date in achieving a physical realization of the Hofstadter model, it had no relation whatsoever to the physical samples in which the integer quantum Hall effect was seen, for which the essentially intractable random potential was the physically-appropriate model, and the apparently-natural problem to study.

Shortly after the TKNN paper was published, Michael Berry discovered his famous geometric phase (Berry, 1984) of adiabatic quantum mechanics. In Berry’s classic example, a spin with quantum number S is aligned along an axis represented by a unit vector $\hat{\Omega}$, with a direction that is slowly changed with time, defining a closed path on the unit sphere that finally returns to its original direction. Berry’s result was that, in addition to the expected change of phase of the state with a rate proportional to its energy, there is an additional “geometric” change of phase that depends only on the geometry of the path, in this case given by the solid angle ω enclosed by the path (the area “enclosed” by the closed path on the surface of the unit sphere) times S . Looking at this more carefully, one sees that the notion of the area enclosed by the path is ambiguous, and the solid angle ω that it subtends is ambiguous up to multiples of 4π , but the physically-meaningful Berry phase factor $\exp iS\omega$ is itself unambiguous because $2S$ is an integer. The influence of Berry’s discovery of the geometric phase on modern developments in quantum theory cannot be overemphasized, and many consider that it deserves to get a fuller exposition in a future lecture in this series.

Both Berry’s work and the TKNN formula were then brought to the attention of the mathematical physicist Berry Simon, who recognized (Simon, 1983) the connection between these formulas whereby the Berry phase could either be viewed as the integral of a “Berry connection” (analogous to the vector potential of electromagnetism) around a path, or by Stokes’ theorem, as the integral of a “Berry flux” or “Berry curvature” through a surface bounded by the path. Furthermore, if the surface is a closed surface with no boundaries, its total Berry curvature or flux must be an integer multiple of 2π , and this integer is a topological invariant, the “first Chern class,” technically of a “ $U(1)$ fiber bundle” (the mathematical characterization of a quantum mechanical wavefunction) on a closed 2D manifold. This theorem is the close analog of the original Gauss-Bonnet theorem for integrals of the intrinsic (Gaussian) curvature over a 2D

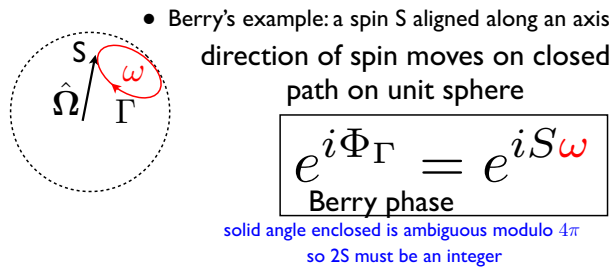


FIGURE 3. Berry phase for the adiabatic evolution of the state of a quantum spin aligned along a moving axis. The Berry phase Φ_Γ is the spin quantum number S times the solid angle subtended by the closed path Γ of the alignment axis $\hat{\Omega}$. After the axis returns to its initial orientation, the final quantum state is the initial state times the factor $\exp i\Phi_\Gamma$ that depends geometrically on the path taken. Since the “solid angle subtended by the path” is ambiguous modulo 4π , $2S$ is topologically required to be an integer (which it is).

surface. If the surface is closed, like a sphere or a doughnut, the Gauss-Bonnet topological invariant counts the number of holes (the “genus” of the surface): it is this precise mathematical analogy that has given rise to the ubiquitous use of the movie showing a bagel or doughnut’s topological equivalence to a coffee cup.

The identification of the TKNN formula as a topological invariant marked the beginning of the recognition that topology would play an important role in classifying quantum states themselves, in addition to the early discovery of the importance of topological excitations in the classical physics of the Berezinsky-Kosterlitz-Thouless transition (see J. Michael Kosterlitz’s Nobel Lecture in this book) This invariant (the “Chern number” or “first Chern class,” given by $\frac{1}{2\pi}$ times the integral of a Berry curvature over a 2D manifold) would remain the only known invariant in quantum condensed matter systems until the 2004 discovery by Kane and Mele (Kane and Mele, 2005) of a new “ Z_2 ” invariant in time-reversal-invariant topological insulators, that led to the current explosion of new experimental and theoretical discoveries about topological states of matter.

The TKNN result was obtained for the bandstructure of electrons in uniform magnetic field with Landau levels that were split into Bloch bands by a periodic potential. In 1988, while analyzing a proposed realization of the “parity anomaly” by Fradkin, Dagotto and Boyanowsky (Fradkin *et al.*, 1986) I realized that the necessary condition for a quantum Hall effect was not a magnetic field, but just broken time-reversal invariance. This perhaps should have been seen as implicit in the TKNN result, but had not apparently been previously noted. I came up with a very simple model (Haldane, 1988) (see Figure 4) based on “a two-dimensional single sheet of graphite” (purely a “toy model” at that time, as the possibility that one day graphene sheets would be made then seemed like

“science fiction”) which I called a model for the “quantum Hall effect without Landau levels,” based on standard Bloch states unlike the esoteric field-dependent ones of the Hofstadter model. This is now called the “quantum anomalous Hall effect” or “Chern insulator.”

This state may also be called the first topological insulator, albeit one with broken time-reversal symmetry. It turns out that in 2D graphene, the “Dirac points” at the corners of the Brillouin zone where the conduction and valence band touch are stable only if both time-reversal and spatial inversion symmetry are unbroken, in which case the Berry curvature vanishes identically, and Berry phase factors for closed paths in the Brillouin zone are topological, with values $\exp i\varphi = \pm 1$, depending on whether their winding numbers around the Dirac points are even or odd. A gapped non-topological insulator state, investigated previously by Semenoff (Semenoff, 1984), results if *spatial inversion symmetry* is broken. In contrast the toy model I devised opens up a gap at the Dirac points to give a quantum Hall state by breaking *time-reversal symmetry*, through giving a chiral phase to second-neighbor hopping between states on the same sublattice. Once the gap opens and breaks the connection between conduction and valence

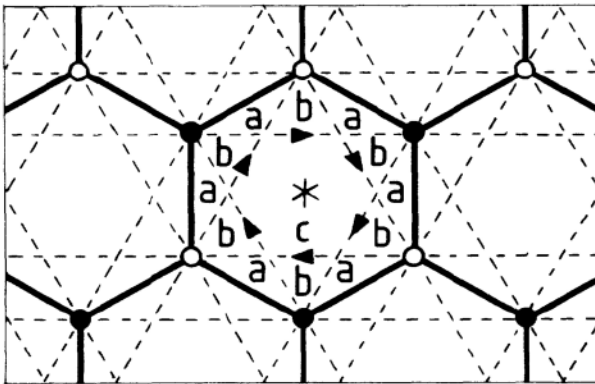


FIGURE 4. The simple graphene-like tight-binding “toy model”(Haldane, 1988) for the “broken-time-reversal topological insulator” or “Chern Insulator” that exhibits a zero-field “quantum anomalous Hall effect.” Electrons “hop” along nearest-neighbor bonds (solid lines) with a real matrix element, and along second-neighbor bonds (dashed lines) with a complex matrix element, which has a positive phase for hopping in the direction of the arrow. Two conjugate copies (one for up-spin, one for down-spin electrons) were later combined by Kane and Mele to model a time-reversal-invariant topological insulator. The complex phases for hopping between second-neighbors introduces broken-time-reversal symmetry, which could come from a ferromagnetically-ordered magnetic dipole at the center (*) of each hexagonal cell, pointing normal to the 2D plane. The dipoles give rise to different magnetic flux through regions *a*, *b*, and *c* of the unit cell, but no net magnetic flux, leaving the standard Bloch structure intact.

bands in the interior of the system, they individually have opposite-sign Chern numbers ± 1 , and unidirectional edge states are present. This is conveniently seen on the “zig-zag” edge, where in the absence of second-neighbor hopping, an zero-energy edge state spans one third of the surface Brillouin zone, connecting the projected Dirac points in a way reminiscent of the recently discovered “Fermi arc” surface states that connect the projected Dirac points of 3D Weyl semi-metals found recently by Ashvin Vishwanath and coworkers (Wan *et al.*, 2011). When a gap opens, whether by breaking inversion symmetry, time-reversal symmetry, or both, the edge states must connect to either the valence or conduction band at each of the now gapped or “massive” Dirac point, leading to four possible outcomes (see Figure 5).

This simple toy model has proved very fruitful: rather surprisingly, while the original model was for charged fermions, it was translated from the language of electrons to that of neutral bosons and a photonic crystal (Haldane and Raghu, 2008), showing how topological “one-way” edge states could occur there too, initiating the growing field of topological photonics, and has been implemented experimentally with microwave-scale photonics.

In 2004, the possibility of a time-reversal-invariant analog of the Hall effect (the “spin-Hall effect”) was under discussion, and a time-reversal invariant (TRI) model was considered by Charles Kane and Eugene Mele (Kane and Mele, 2005), who combined two conjugate copies of my model, one for spin-up electrons for which the valence band had Chern number ± 1 and one for spin-down electrons where the valence band had the opposite value ∓ 1 ; on the edges, spin-up and spin-down edge modes propagated in opposite directions. Since the total Chern

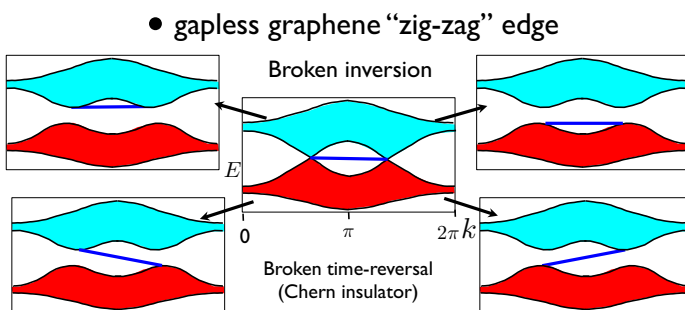


FIGURE 5. “Zig-Zag” edge of graphene after perturbation by terms that break inversion or time-reversal symmetry. The unperturbed edge has an edge state joining the projections of the two Dirac points where the filled valence band (red) touches the empty conduction bands (green). When a gap is induced by the perturbation, there are four ways the edge-state can be connected, two of which are topological, and connect conduction and valence bands.

number of the valence band vanished, there was no quantum Hall effect. Naively, it might have been expected that the gapless edge modes were not protected from backscattering and mixing, thus becoming gapped, if spin-non-conserving Rashba-type spin-orbit coupling was added to the system. However Kane and Mele discovered by a numerical calculation that, so long as time-reversal invariance was unbroken, the edge modes were in fact protected by a previously-unexpected “ Z_2 ” topological invariant related to Kramers degeneracy. This new invariant had a 3D generalization discovered independently and simultaneously in 2007 by Joel Moore and Leon Balents (Moore and Balents, 2007), Rahul Roy (Roy, 2009), and Liang Fu, Kane and Mele (Fu *et al.*, 2007), which led to the experimental discovery of the 3D time-reversal-invariant topological insulators (TI). This finally led to the reported experimental realization (Chang *et al.*, 2013) by QiKun Xue’s group at Tsinghua University, Beijing, of the quantum anomalous Hall effect in thin films of TRI TIs which had been doped with magnetic material.

I now turn to the other (1981) discovery recognized by this Nobel prize: the novel quantum spin liquid states of the one-dimensional integer-spin antiferromagnets, which (for odd integral spin) have recently been classified by Xiao-Gang Wen and collaborators (Chen *et al.*, 2013) as “symmetry protected topological states” (SPT states), where the protective symmetries are time-reversal invariance and spatial inversion symmetry. The conventional magnetic ground states generally studied prior to 1981 were typically unentangled states, usually with long-range magnetic order, that could be modeled as a direct product of independent states on each sites, such as a ferromagnet ($\dots \uparrow \uparrow \uparrow \uparrow \uparrow \dots$) or a Néel antiferromagnet ($\dots \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \dots$). The spin configurations shown have spins aligned parallel or antiparallel to the z -axis, but in the case of Heisenberg (isotropic) magnets these states spontaneously break rotational symmetry, and the alignment axis can point in any direction. In the case of the Heisenberg ferromagnet, the alignment direction is the direction of a macroscopic conserved angular momentum vector, and the conservation law for angular momentum of a rotationally-invariant system protects the ferromagnetic “order parameter” (the alignment direction) against deviation by zero-point fluctuations.

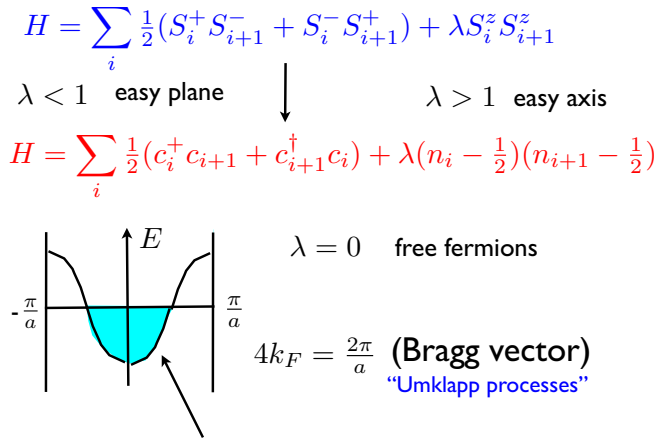
However, in the antiferromagnetic case, there is no conservation law to give protection against zero-point fluctuations, The celebrated Mermin-Wagner theorem that posed the key paradox in the case-of the finite temperature Kosterlitz-Thouless transition provides a similar result for quantum systems in one spatial dimension: without protection by a conservation law, the ground state of a quantum system with a continuous symmetry cannot exhibit long-range order of an order-parameter that breaks that symmetry. In higher dimensions, Heisenberg

systems can exhibit antiferromagnetic broken symmetry ground states with gapless collective Goldstone-mode excitations known as (antiferromagnetic) spin waves that are small harmonic fluctuations of the Néel order-parameter around its uniform ground state configuration. But, if the assumption of long-range Néel antiferromagnetic order is made in the case of the one-dimensional spin- S antiferromagnet, it is easily found that the effect of the harmonic zero-point fluctuations would be to destroy the assumed long-range order.

At this point the power of exact (but not fully understood) mathematical results to sow confusion enters the story! In 1931, before he went on to discover how nuclear fusion powered the sun (and later to become David Thouless's thesis advisor at Cornell), Hans Bethe also worked on the one-dimensional Heisenberg chain as a "toy model" for magnetism, and discovered a remarkable "Ansatz" (Bethe, 1931) that provided exact solutions for eigenstates of the 1D model with $S = \frac{1}{2}$ and nearest-neighbor exchange, allowing the eigenvalue spectrum to be explicitly obtained. Unfortunately, it took more than sixty years for the underlying special mathematical structure of the model to be understood, and in the 1970s, only energy levels and thermodynamic properties could be extracted from the exact solutions, but not the correlation functions. However, the spectrum of low-energy eigenvalues superficially resembled the predictions of spin-wave theory with the only apparent change being that the speed of long-wavelength spin waves differed from the predictions of spin-wave theory by a factor of $\frac{1}{2}\pi$.

While the details of Bethe's Ansatz were somewhat arcane and mysterious, this was generally taken as confirmation that the spin-wave description was more-or-less correct despite the known destruction of true long-range order by quantum effects. In fact, we now know that the elementary excitations of the model that Bethe solves have *no relation whatsoever to spin waves*: they are spin- $\frac{1}{2}$ topological excitations (Faddeev and Takhtajan, 1981) that are created in pairs, and now known as "spinons," but even in the 1970s it ought to have been noticed that, when expressed in terms of the velocity of long wavelength excitations, the specific heat predicted by spin-wave theory was exactly twice the exact result extracted from the Bethe Ansatz, implying no relation of any kind between the spin-wave theory and low-energy excitations of Bethe's solvable model.

To get around the long-standing intractability of the problem of extracting correlation functions from Bethe's solution, new techniques for treating the problem emerged in the early 1970's from the work of Alan Luther and Ingo Peschel. Again old work (even older than Bethe's!) was important: they used the Jordan-Wigner (Jordan and Wigner, 1928) transformation that maps the one-dimensional magnet with nearest-neighbor exchange into a model of spinless



Half-filled band (in zero magnetic field)

FIGURE 6. The Jordan-Wigner transformation maps the $S = \frac{1}{2}$ Heisenberg chain with zero magnetization into a half-filled interacting band of spinless fermions, where $4k_F$ is a Bragg vector.

fermions that move in one dimension by hopping between nearest neighbor sites on the lattice, with interactions between particles on neighbor sites. When the Heisenberg exchange coupling $\vec{S}_n \cdot \vec{S}_{n+1}$ is decomposed into $J^x S_n^x S_{n+1}^x + J^y S_n^y S_{n+1}^y + J^z S_n^z S_{n+1}^z$, with $J^x = J^y = J^z$, the $S = \frac{1}{2}$ “quantum XY” model with $J^z = 0$ is mapped into a non-interacting free-fermion model that can be completely and explicitly solved to extract all physical properties.

In the mid-1960s, Joaquin Luttinger (Luttinger, 1963) had noticed that a “toy model” of interacting spinless fermions with a linear Dirac-like dispersion and an interaction restricted to low momentum-transfer forward scattering should be solvable using the “Tomonaga bosons” found by Sin-itiro Tomonaga (Tomonaga, 1950). There were problems with Luttinger’s solution, which was subsequently elucidated by Daniel Mattis and Elliott Lieb (Mattis and Lieb, 1965), and from this came the remarkable “bosonization” technique (representation of one-dimensional fermions in terms of Tomonaga’s harmonic oscillator modes) explicitly formulated by Schotte and Schotte (Schotte and Schotte, 1969) in their 1969 simplified treatment of the “X-ray edge singularity” problem.

In 1975, Luther and Peschel (Luther and Peschel, 1975) adapted the new “bosonization” techniques to treat the easy-plane antiferromagnet with non-zero $J^z = \lambda |J^y|$, with $|\lambda| < 1$, which they mapped into a “(1+1)-dimensional” effective quantum field theory could be treated by the “bosonization” mapping to a harmonic oscillator problem. This treatment was precisely equivalent (after a “Wick

rotation” from (1+1)-dimensional Lorentz-invariant space-time to 2-dimensional Euclidean space) to the low-temperature “topologically-ordered” phase of the classical 2D XY model which Kosterlitz and Thouless were also studying at that time, with Néel correlations that decayed algebraically with non-universal power laws, where for large $|n - n'|$,

$$\langle S_n^x S_{n'}^x \rangle = \langle S_n^y S_{n'}^y \rangle \propto (-1)^{n-n'} |n - n'|^{-\eta}, \quad \langle S_n^z S_{n'}^z \rangle \propto (-1)^{n-n'} |n - n'|^{-\eta^{-1}} \quad (3)$$

where η varied with the coupling-constant ratio λ . Furthermore, introducing full “XYZ” anisotropy ($J^x \neq J^y$) maps the model to a massive field theory (the “sine-Gordon” model) with a excitation gap that depends algebraically on $J^x - J^y$ with an exponent fixed by η .

By that time Bethe’s exact solution of the $S = \frac{1}{2}$ isotropic Heisenberg “XXX” model ($J^x = J^y = J^z$) had been extended to the full XYZ model by Rodney Baxter, following the identification of the Yang-Baxter algebra as the key ingredient that allowed Bethe’s Ansatz to solve the model. Luther and Peschel were able to use this to indirectly obtain the value of the correlation exponent η as a function of λ for the easy plane “XXZ” model ($|\lambda| \leq 1$). They found that for positive (antiferromagnetic) J^z , η increases from $\frac{1}{2}$ at the fully-solvable “free-fermion” XY point with $J^z = 0$, reaching the consistent value $\eta = \eta^{-1} = 1$ at the antiferromagnetic Heisenberg “XXX” point $\lambda = 1$, while for negative (ferromagnetic) J^z , it decreases to zero when $\lambda = -1$, where the ground state develops long-range order with a conserved order parameter. Notably, the Luther-Peschel field-theory treatment failed to explain the gap that opens for $\lambda > 1$, when the model changes from an easy-plane to an easy-axis antiferromagnet.

In 1979 I was working on the precise formulation of the bosonization method and found (Haldane, 1981b) that the zero-momentum modes of the fermion density needed to be represented by action-angle variables as opposed to Tomonaga’s harmonic oscillator modes which represented the modes carrying finite momentum. These action-angle degrees of freedom are topological in nature, and resolved the “mystery” of how one-dimensional fermions could apparently be represented in terms of “bosons” (harmonic oscillator modes): the representation in fact is constructed using harmonic oscillators *plus* topological winding-number degrees of freedom. This meant that the detailed structure of the excitation spectrum of a spinless fermion model with periodic boundary conditions contained two types of topological excitations (separate winding numbers of left- and right-moving fermion fields) as well as Tomonaga’s sound-wave modes.

Knowledge of the energies of the two topological excitations fixed not only the speed of sound, which could be independently checked, but also the correlation exponent η , and applying this to the Bethe Ansatz solution of the XXZ model in zero field (or the equivalent Jordan-Wigner fermion model with a half-filled band) for which Luther and Peschel had indirectly found the exact value of the exponent η as a function of the couplings, I was able to confirm that the new expressions in terms of winding-number energies were also consistent, correct, and quite general.

This opened up by the possibility of extracting exact correlation exponents from Bethe Ansatz solutions of some models exhibiting one-dimension criticality by using the energies of their various topological excitations to fit them to what I called an effective “Luttinger liquid” (Haldane, 1981b) (or perhaps more properly a “Tomonaga-Luttinger liquid”) modeled by a Luttinger model. These developments occurred before the later appearance of more powerful (1+1)-dimensional conformal field theory methods, and “Luttinger liquids” turn out to be systems decomposable into Abelian representations of the Virasoro algebra, with the constraints of Lorentz invariance removed.

When I applied this new picture to the the full parameter space of the Bethe-Ansatz solutions of the XXZ spin chain (which required numerical solution of the Bethe Ansatz integral equations away from half-filling of the fermion bands) it became immediately obvious from inspection of the results that the missing ingredient in Luther and Peschel’s work was the omission of the “Umklapp” process by which, at half-filling of the band (where $4k_F$ is a Bragg vector), so scattering processes where the momentum changes by $4k_F$ allow two low-energy “left-moving” electrons (each with momentum near $-k_F$) to scatter into two low-energy right-moving electron states, each with momentum near k_F .

At first sight this should be represented by a term $\Psi_R^\dagger(x)\Psi_R^\dagger(x)\Psi_L(x)\Psi_L(x)$, but this is ruled out by the Pauli principle, which is presumably why Umklapp was not considered in the original work by Luther and Peschel, but the next-order term $(\Psi_R^\dagger(x)\partial_x\Psi_R^\dagger(x))(\Psi_L(x)\partial_x\Psi_L(x))$ is allowed, and when “bosonized” becomes $\cos 2\theta \equiv \cos 2(\phi_R(x) - \phi_L(x))$. In the quantum analog of the Berezinsky-Kosterlitz-Thouless (BKT) transition, this is a *double-vortex unbinding transition*, which is allowed, but the standard *single-vortex unbinding transition* is forbidden by momentum conservation. The translation of the usual single-vortex BKT process from classical 2D to quantum (1+1)D would be represented by a term $\cos\theta$ which becomes “relevant” (causing a gap to open) when $\eta > \frac{1}{4}$. The generalization of this is that a $\cos m\theta$ term becomes relevant when $\eta > \frac{1}{4}m^2$, which is perfectly consistent with the double-vortex term $\cos 2\theta$ becoming

relevant (in the absence of the single-vortex term) exactly at the isotropic XXX point when $\eta = 1$.

This missing ingredient completed the field-theoretic picture of the $S = \frac{1}{2}$ begun by Luther and Peschel. It also removed the the apparent “special” nature of the $S = \frac{1}{2}$ model which seemed to come from its mapping to a fermion model. The bosonization now provided a representation in terms of two “chiral” (left-moving and right-moving) topological winding number fields $\varphi_L(x)$ and $\varphi_R(x)$, without any obvious relation to the value of the spin S of the underlying spin chain.

A planar “XY” spin can be visualized as a “compass needle” that points in a 2D direction $(\cos(\varphi(x)), \sin(\varphi(x)))$, and if it obeys a periodic boundary condition on a circle of circumference L , then $\varphi(x + L) = \varphi(x) + 2\pi W$ where the “winding number” W is a topological invariant that cannot change if the field $\varphi(x)$ varies smoothly with x . In the classical 2D XY model, $\varphi(x, y)$ is a smooth function except at singular points (x_0, y_0) which are the centers of vortices. In the quantum (1+1)D model these become space-time points (x_0, t_0) representing tunneling events (which have been called “instantons”) at which the winding number changes, through a singular process that occurs briefly at a 1D space point x_0 and during an instant of time near t_0 .

It turned out that for a spin- S easy-plane spin chain with zero magnetization along the z -axis, the usual “single-vortex” BKT “instanton” process is generically present, but is forbidden by an exact *quantum interference* process if $2S$ is odd. This highlights a difference between the classical statistical mechanics of the 2D BKT transition and the (1+1)D quantum version. In the classical 2D model, the

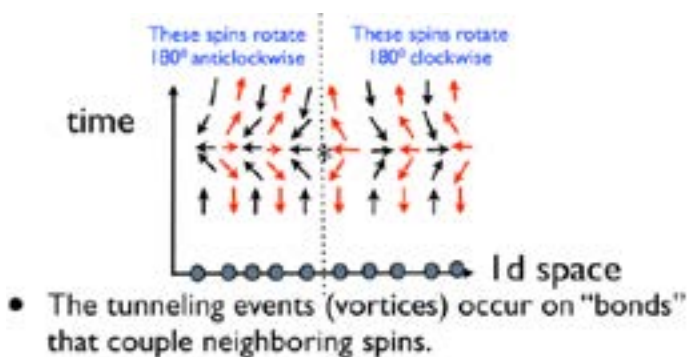


FIGURE 7. In (1+1)D space-time, the analog of the 2D vortex is an “instanton” tunnelling process where the topological winding number of the easy-plane spin-chain changes. This process is centered on a “bond” between consecutive sites on which the local Néel order breaks down for a short time interval.

strength of the vortex term in the Boltzmann factor is a real positive fugacity factor, but in the quantum (1+1)D model, it is a complex amplitude for tunneling between topologically-different configurations with different winding number, and is real-positive or negative in time-reversal-invariant models. This means that quantum interference between competing instanton processes can occur.

In this case the tunneling process is centered at the midpoint of a “bond” between two neighboring spins. Assuming the spin chain is invariant under spatial translation by one site, the *magnitude* of the amplitude for the tunneling process must be the same independent of which bond it is centered on. But when two such processes on consecutive bonds are compared, the main difference is that one spin that rotated 180° clockwise now rotates 180° anticlockwise, so the two processes differ by a net rotation of one spin by 360° , with the histories of all other spins essentially identical. The fundamental difference between a spin where $2S$ is even and one where $2S$ is odd is that in the latter case, there is quantum state has a sign change as a result of the rotation. This means that, providing the exchange energy is the same on all bonds, there is destructive interference between instanton tunneling events on neighboring bonds if $2S$ is odd, but constructive interference if $2S$ is even.

This provides the “topological” explanation of why the instanton process that becomes relevant as the anisotropy of the spin- $\frac{1}{2}$ XXZ chain changes from easy-plane to easy axis corresponds to a *double vortex* of the BKT transition. It only drives the instability of the topologically-ordered easy-plane phase because the dominant *single vortex* process is canceled by destructive interference when $2S$ is odd. However, for integer S it is present, and the BKT transition will occur once the correlation exponent rise to the limiting value $\eta = \frac{1}{4}$ when tunneling between states with different winding number becomes relevant, topological order breaks down, and a gap in the excitation spectrum opens up. At this critical point the Néel correlations of $(S_n^x S_{n'}^x)$ and $(S_n^y S_{n'}^y)$ fall off much slower than those of $(S_n^z S_{n'}^z)$ implying that the transition happens before the isotropic Heisenberg point is reached. It is also a transition to a *unique* (singlet) ground state, while the double-vortex process conserves winding-number modulo 2, and leads to a two-fold degenerate (doublet) ground state when it becomes relevant.

From these results, it became clear that the progression from easy-plane to easy-axis models was quite different in the two cases of integer- S and half-odd-integer- S antiferromagnets. As λ increases, the chain with $2S$ odd has a direct “double-BKT” transition at $\lambda = 1$ from the topologically-ordered gapless easy-plane antiferromagnet with $\lambda < 1$ to the gapped easy-axis antiferromagnet with a doublet broken-symmetry Ising-Néel ground state. In contrast, the chain with even $2S$ has a standard BKT transition at $\lambda = \lambda^c < 1$ to a singlet gapped

spin-liquid state with no broken symmetry, followed by a second Ising-type transition at $\lambda = \lambda^c > 1$ to the easy-axis Ising-Néel state.

These arguments exposed a fundamental topological difference between antiferromagnetic Heisenberg (isotropic) quantum spin- S chains with $2S$ even and those with $2S$ odd, which contradicted the then-prevailing belief that the value of S entered as a continuous parameter as an expansion in powers of S^{-1} analogous to a semiclassical expansion in powers of \hbar . In this view, the asymptotic long-distance behavior of $\langle \vec{S}_n \cdot \vec{S}_{n'} \rangle$ would behave as $(-1)^{n-n'} |n - n'|^{-\eta}$, where $\eta(S^{-1})$ was a smooth function of S^{-1} that vanishes as $S^{-1} \rightarrow 0$.

My apparently-heretical 1981 claim, that there was a fundamental difference between one-dimensional quantum antiferromagnets with integer and half-odd-integer S , was presumably not well-enough explained, and the original paper (Haldane, 1981a) was rejected by a number of journals, and referred to by sceptics as a “conjecture,” a description that seems to have stuck! By the time the paper was finally published (Haldane, 1983a), it had been significantly rewritten to emphasise the isotropic Heisenberg case, and the original preprint was eventually apparently lost, as this was years before preprints were stored on the internet. Happily, I recently recovered a copy that had been preserved by Jenő Sólyom, and placed it in the arXiv repository (Haldane, 1981a) for historical interest. Subsequently numerical exact diagonalization studies by Botet and Jullien (Botet and Jullien, 1983) found evidence for it, and finally, neutron scattering studies by Bill Buyers (Buyers *et al.*, 1986) on the quasi-one dimensional organic Nickel compound NENP provided experimental confirmation that the ground state of the spin-1 antiferromagnet was a singlet with an excitation gap.

The underlying reason that my 1981 result was so unexpected was that the spin-liquid state of the integer spin-1 chain was an early example of “topological quantum matter.” The discovery predated Berry’s 1983 discovery of the Berry phase, which in spin systems confirmed that the spin quantum number S had a topological role which relied on the value of $2S$ being an integer. Initially, from the standard Hamiltonian formulation used by condensed-matter physicists, it seemed mysterious that there seemed to be two distinct ways to apply quantum mechanics to a continuum field theory description of quantum antiferromagnetic spin chains, the “ $O(3)$ non-linear sigma model,” one for half-odd-integer spins, and the other for integer spins. In 1983, a very useful lead came from a discussion I had with Edward Witten, who mentioned that in the Lagrangian formulation favored by particle physicists, the sigma model could have an additional “topological term,” which disappeared in the Hamiltonian formulation, and had no effect in the classical limit. This term is parameterized by an angle θ ; and it was easy to use a formulation in terms of the Berry phases of the paths

traced out by individual spins to show that this angle was $2\pi S$, taking the value 0 modulo 2π for integers spins, and π modulo 2π for half-odd-integer spins (these are the only two values compatible with time-reversal symmetry). This angle parameter is related to the “axion angle” introduced in high-energy physics in connection with the “strong-CP-violation” problem, and more recently in the electrodynamic description of “strong topological insulators” by Xiao-Liang Qi, Taylor Hughes and Shoucheng Zhang (Qi *et al.*, 2008), where the analogous “topological angle” takes the value $\theta = 0$ for non-topological TRI insulators, and $\theta = \pi$ for the strong 3D TRI topological insulators. The discovery of the “theta-term” in the Lagrangian form of the field theory of the one-dimensional anti-ferromagnets seems to mark the time after which the Lagrangian formulation started to become ubiquitous in theoretical quantum condensed-matter physics, and it is now a standard tool that complements Hamiltonian descriptions.

A simple model state that captures the essence of the gapped integer- S 1D antiferro-magnet was subsequently discovered by Ian Affleck, Tom Kennedy, Hal Tasaki, and Elliot Lieb (Affleck *et al.*, 1987), which is also the exact ground state of a modified “toy model” (the “AKLT model”), which is particularly revealing, as it shows up the novel nature of quantum entanglement in the topological state. In this picture, a spin-1 object is viewed as a symmetric state of two spin- $\frac{1}{2}$ “half-spins,” each of which can form an entangled singlet “valence bond” state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad (4)$$

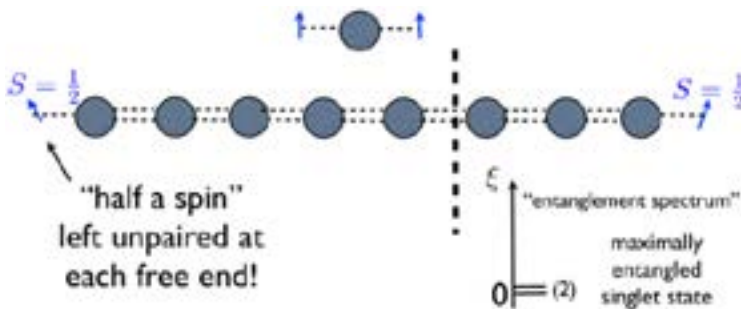


FIGURE 8. The $S = 1$ AKLT state treats each spin as a symmetric combination of two $S = \frac{1}{2}$ “half-spins,” one of which forms a singlet valence bond with a “half-spin” of the neighbor to the right, the other with the neighbor to the left. An unused spin- $\frac{1}{2}$ is left at each open end of the chain, and the “entanglement spectrum” consists of a single doublet.

by pairing with one of the half-spins of each neighbor. If the magnetic chain has free ends (*i.e.*, is “open”), this leaves an unpaired spin- $\frac{1}{2}$ at each end of the chain. This model also reveals the essentially “entangled” nature of the state: if the chain is cut in two, unpaired spin- $\frac{1}{2}$ degrees of freedom appear on either side of the cut, and the model state has a very simple characteristic “entanglement spectrum” (Li and Haldane, 2008) of a single spin- $\frac{1}{2}$ doublet. The feature that all states in the entanglement spectrum are doublets, and that free ends of a long open spin-1 chain carry local spin- $\frac{1}{2}$ degrees of freedom is true for all states in the same topological class as the AKLT model, including the standard spin-1 Heisenberg antiferromagnet that I originally studied. (See Figure 8.)

The edges of the (integer) spin- S chain have local spin- $\frac{1}{2}S$ degrees of freedom, but since the elementary gapped bulk excitations are spin-1 magnons which can bind to the edge, the edge spins are topologically protected only when S is an *odd* integer. The final classification (Chen *et al.*, 2013) is that only the odd-integer- S state is a “symmetry protected topological state” (SPT state) protected by either time-reversal symmetry or spatial inversion, with a generic two-fold degeneracy of states in the entanglement spectrum.

Over the years, studies of topological state of the $S = 1$ Heisenberg antiferromagnet have been remarkable fruitful. The detailed study of its topological stability was the starting point that led a unified classification of SPT states in both one dimension and higher dimensions by Xiao-Gang Wen and collaborators (Chen *et al.*, 2013). In addition, its entanglement spectrum lies at the heart of the “density-matrix renormalization group” (White, 1992) and “matrix-product state” techniques that were in part developed for testing and verifying the so-called “Haldane conjecture.” The features of unexpected topologically-protected edge states recur again and again in connection with “topological state of matter,” for example in the “Majorana modes” that appear at the edge of topological superconducting wires, where the simple “toy model” introduced by Kitaev (Kitaev, 2001) plays a similar role to the AKLT model, and are now considered to be a possible platform for future topological quantum information processing. It is surprising how rich the developments stemming from the surprise discovery of topological phases of matter around 1980 has been.

Looking back at how this new field of topological quantum matter has developed since the initial discoveries in about 1980, I am struck by how important the use of stripped down “toy models” has been in discovering new physics. It also used to be thought that one-dimensional models were just “homework exercises” to be carried out before tackling the “real” three dimensional systems. In fact, partly because the effects of quantum fluctuations are more dramatic in

low dimensions, we have found many interesting phenomena, in in doing so, a whole new way to look at condensed matter, and the exotic “topological states” that quantum mechanics make possible.

It has been my privilege to have been able to participate in opening up this field, to which many others have added amazing discoveries, and which has led to dreams of new quantum information technologies. I thank the Royal Swedish Academy of Sciences for honoring my co-Laureates and myself, and indeed our exciting subfield of physics.

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