

TOPOLOGY IN PHYSICS*

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The phenomenon of quantum number fractionalization is explained. The relevance of non-trivial phonon field topology is emphasized.

1. Introduction

Discussions of the spatial forms of physical materials use in a natural way geometrical and topological concepts. It is to be expected that arrangements of matter should form patterns that are described by pre-existing mathematical structures drawn from geometry and topology. But theoretical physicists also deal with abstract entities, which do not have an actual material presence. Still geometrical and topological considerations are relevant to these ephemeral theoretical constructs. I have in mind fields, both classical and quantum, which enter into our theories of fundamental processes. These fields $\phi(x)$ provide a mapping from a “base” space or space-time on which they are defined into the field “target” manifold on which they range. The base and target spaces, as well as the mapping, may possess some non-trivial topological features, which affect the fixed time description and the temporal evolution of the fields, thereby influencing the physical reality that these fields describe. Quantum fields of a quantum field theory are operator valued distributions whose relevant topological properties are obscure. Nevertheless, topological features of the corresponding classical fields are important in the quantum theory for a variety of reasons: (i) Quantized fields can undergo local (space-time dependent) transformations (gauge transformations, coordinate diffeomorphisms) that involve classical

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functions whose topological properties determine the allowed quantum field theoretic structures. (ii) One formulation of quantum field theory uses a functional integral over classical fields, and classical topological features become relevant. (iii) Semi-classical (WKB) approximations to the quantum theory rely on classical dynamics, and again classical topology plays a role in the analysis.

Topological effects in quantum electrodynamics were first appreciated by Dirac in his study of the quantum mechanics for (hypothetical) magnetic monopoles. This analysis leads directly to contemporary analysis of Yang-Mill theory – the contemporary generalization of Maxwell’s electrodynamics – and has yielded several significant results: the discovery of the θ -vacuum angle; the recognition that c -number parameters in the theory may require quantization for topological reasons (like Dirac’s monopole strength); the realization that the chiral anomaly equation is just the local version of the celebrated Atiyah-Singer index theorem.

Here I shall not describe the Yang-Mills investigations; they are too technical and too specialized for this general audience. Rather I shall show you how a topological effect in a condensed matter situation leads to charge fractionalization. This phenomenon has a physical realization in 1-dimensional (lineal) polymers, like polyacetylene, and in 2-dimensional (planar) systems, like the Hall effect.

The polyacetylene story is especially appealing, because it can be told in several ways: in pictorial terms which only involves counting, or in the first quantized formalism for quantum mechanical equations, or in the second quantized formalism of a quantum field theory ¹.

2. The Polyacetylene Story (Counting Argument)

Polyacetylene is a material consisting of parallel chains of carbon atoms, with electrons moving primarily along the chains, while hopping between chains is strongly suppressed. Consequently, the system is effectively 1-dimensional. The distance between carbon atoms is about 1\AA .

If the atoms are considered to be completely stationary, *i.e.* rigidly attached to their equilibrium lattice sites, electron hopping along the chain is a structureless phenomenon. However, the atoms can oscillate around their rigid lattice positions for a variety of reasons, like zero-point motion, thermal excitation, etc. It might be thought that these effects merely give rise to a slight fuzzing of the undistorted-lattice situation.

In fact this is not correct; something more dramatic takes place. Rather

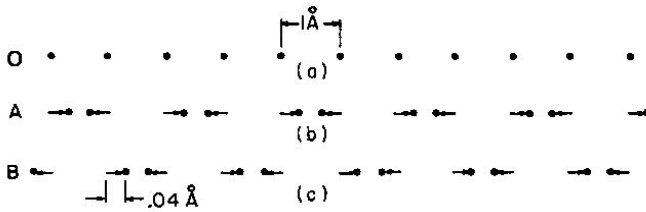


Figure 1. (a) The rigid lattice of polyacetylene; (O) the carbon atoms are equally spaced 1 Å apart. (b), (c) The effect of Peierls' instability is to shift the carbon atoms .04Å to the right (A) or to the left (B), thus giving rise to a double degeneracy.

than oscillating about the rigid-lattice sites, the atoms first shift a distance of about .04 Å and then proceed to oscillate around the new, slightly distorted location. That this should happen was predicted by Peierls, and is called the Peierls instability. Due to reflection symmetry, there is no difference between a shift to the right or a shift to the left; the material chooses one or the other, thus breaking spontaneously the reflection symmetry, and giving rise to doubly degenerate vacua, called A and B.

If the displacement is described by a field ϕ which depends on the position x along the lattice, the so-called phonon field, then Peierls' instability, as well as detailed dynamical calculations indicate that the energy density $V(\phi)$, as a function of constant ϕ , has a double-well shape. The symmetric point $\phi = 0$ is unstable; the system in its ground state must choose one of the two equivalent ground states $\phi = \pm |\phi_0| = \pm .04\text{Å}$. In the ground states, the phonon field has uniform values, independent of x .

By now it is widely appreciated that whenever the ground state is degenerate there frequently exist additional stable states of the system, for which the phonon field is non-constant. Rather, as a function of x , it interpolates, when x passes from negative to positive infinity, between the allowed ground states. These are the famous solitons, or kinks. For polyacetylene they correspond to domain walls which separate regions with vacuum A from those with vacuum B, and vice versa. One represents the chemical bonding pattern by a double bond connecting atoms that are closer together, and the single bond connecting those that are further apart.

Consider now a polyacetylene sample in the A vacuum, but with two solitons along the chain. Let us count the number of links in the sample without solitons and compare with number of links where two solitons are present. It suffices to examine the two chains only in the region where they differ, *i.e.* between the two solitons. Vacuum A exhibits 5 links, while the

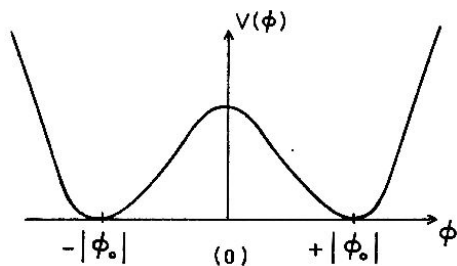


Figure 2. Energy density $V(\phi)$, as a function of a constant phonon field ϕ . The symmetric stationary point, $\phi = 0$, is unstable. Stable vacua are at $\phi = +|\phi_0|$, (A) and $\phi = -|\phi_0|$, (B).

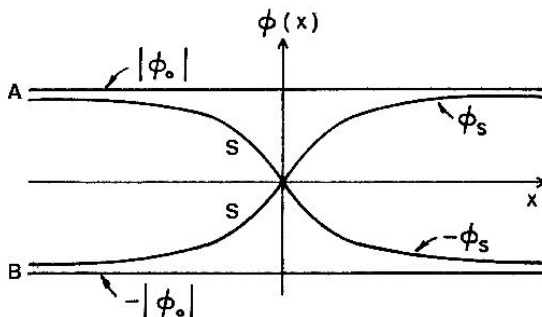


Figure 3. The two constant fields, $\pm |\phi_0|$, correspond to the two vacua (A and B). The two kink fields, $\pm \phi_s$, interpolate between the vacua and represent domain walls.

addition of two solitons decreases the number of links to 4. The two soliton state exhibits a deficit of one link. If now we imagine separating the two solitons a great distance, so that they act independently of one another, then each soliton carries a deficit of half a link, and the quantum numbers of the link, for example the charge, are split between the two states. This is the essence of fermion fractionization.

It should be emphasized that we are not here describing the familiar situation of an electron moving around a two-center molecule, spending “half” the time with one nucleus and “half” with the other. Then one might say that the electron is split in half, on the average; however fluctuations in any quantity are large. But in our soliton example, the fractionization is without fluctuations; in the limit of infinite separation one achieves an eigenstate with fractional eigenvalues.

We must however remember that the link in fact corresponds to two states: an electron with spin up and another with spin down. This doubling

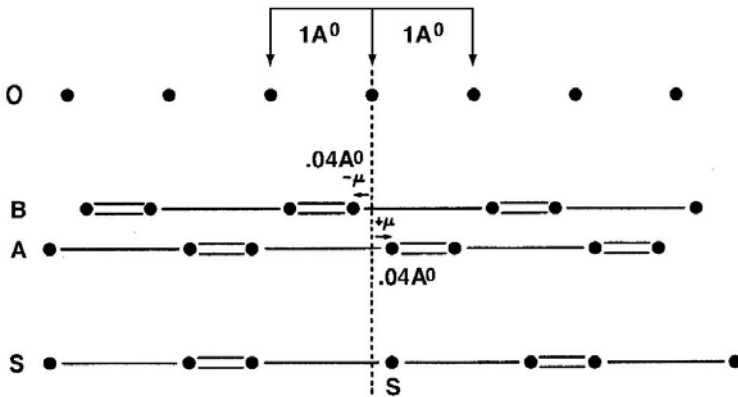


Figure 4. Polyacetylene states. The equally spaced configuration (O) possesses a left-right symmetry, which however is energetically unstable. Rather in the ground states the carbon atoms shift a distance μ to the left or right, breaking the symmetry and producing two degenerate vacua (A, B). A soliton (S) is a defect in the alteration pattern; it provides a domain wall between configurations (A) and (B).

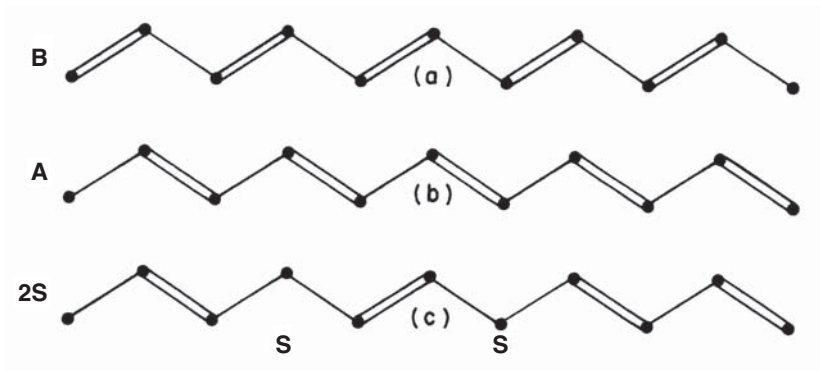


Figure 5. (a), (b) Pattern of chemical bonds in vacua A and B. (c) Two solitons inserted into vacuum A.

obscures the dramatic charge $\frac{1}{2}$ effect, since everything must be multiplied by 2 to account for the two states. So in polyacetylene, a soliton carries a charge deficit of one unit of electric charge. Nevertheless charge fractionization leaves a spur: the soliton state has net charge, but no net spin, since all of the electron spins are paired. If an additional electron is inserted into the sample, the charge deficit is extinguished, and one obtains a neutral state, but now there is a net spin. These spin-charge assignments (charged

– without spin, neutral – with spin) are unexpected, but in fact have been observed, and provide experimental verification for the soliton picture and fractionalization in polyacetylene.

Notice that in this simple counting argument no mention is made of topology. This feature emerges only when an analytic treatment is given. I now turn to this.

3. The Polyacetylene Story (Quantum Mechanics)

I shall now provide a calculation which shows how charge 1/2 arises in the quantum mechanics of fermions in interaction with solitons. The fermion dynamics are governed by an one-dimensional Dirac Hamiltonian, $H(\phi)$, which also depends on a background phonon field ϕ , with which the fermions interact. The Dirac Hamiltonian arises not because the electrons are relativistic. Rather it emerges in a certain well-formulated approximation to the microscopic theory, which yields a quantal equation that is a 2×2 matrix equation, like a Dirac equation. In the vacuum sector, ϕ takes on a constant value ϕ_0 , appropriate to the vacuum. When a soliton is present, ϕ becomes the appropriate, static soliton profile ϕ_s . We need not be any more specific. We need not insist on any explicit soliton profile. All that we require is that the topology [*i.e.* the large distance behavior] of the soliton profile be non-trivial.

In the present lineal case the relevant topology is that infinity corresponds to two points, the end points of the line, and the phonon field in the soliton sector behaves differently at the points at infinity.

To analyze the system we need the eigenmodes, both in the vacuum and soliton sectors.

$$H(\phi_0)\psi_E^v = E\psi_E^v \tag{1}$$

$$H(\phi_s)\psi_E^s = E\psi_E^s \tag{2}$$

The Dirac equation is like a matrix-valued “square root” of the wave equation. Because a square root is involved, there will be in general negative energy solutions and positive energy solutions. The negative energy solutions correspond to the states in the valence band; the positive energy ones, to the conduction band. In the ground state, all the negative energy levels are filled, and the ground state charge is the integral over all space of the charge density $\rho(x)$, which in turn is constructed from all the negative

energy wave functions.

$$\rho(x) = \int_{-\infty}^0 dE \rho_E(x), \quad \rho_E(x) = \psi_E^*(x) \psi_E(x) \quad (3)$$

Of course integrating (3) over x will produce an infinity; to renormalize we measure all charges relative to the ground state in the vacuum sector. Thus the soliton charge is

$$Q = \int dx \int_{-\infty}^0 dE \{\rho_E^s(x) - \rho_E^v(x)\}. \quad (4)$$

Eq. (4) may be completely evaluated without explicitly specifying the soliton profile, nor actually solving for the negative energy modes, provided H possesses a further property. We assume that there exists a conjugation symmetry which takes positive energy solutions of (1) and (2) into negative energy solutions. (This is true for polyacetylene.) That is, we assume that there exists a unitary 2×2 matrix M , such that

$$M\psi_E = \psi_{-E}. \quad (5)$$

An immediate consequence, crucial to the rest of the argument, is that the charge density at E is an even function of E .

$$\rho_E(x) = \rho_{-E}(x) \quad (6)$$

Whenever one solves a conjugation symmetric Dirac equation, with a topologically interesting background field, like a soliton, there always are, in addition to the positive and negative energy solutions related to each other by conjugation, self-conjugate, normalizable zero-energy solutions. That this is indeed true can be seen by explicit calculation. However, the occurrence of the zero mode is also predicted by very general mathematical theorems about differential equations. These so-called ‘‘index theorems’’ count the zero eigenvalues, and insure that the number is non-vanishing whenever the topology of the background is non-trivial. We shall assume that there is just one zero mode, described by the normalized wave function ψ_0 .

To evaluate the charge Q in (4), we first recall that the wave functions are complete, both in the soliton sector and in the vacuum sector.

$$\int_{-\infty}^{\infty} dE \psi_E^*(x) \psi_E(y) = \delta(x - y) \quad (7)$$

As a consequence, it follows that

$$\int_{-\infty}^{\infty} dE [\rho_E^s(x) - \rho_E^v(x)] = 0. \quad (8a)$$

In the above completeness integral over all energies, we record separately the negative energy contributions, the positive energy contributions, and for the soliton, the zero-energy contribution. Since the positive energy charge density is equal to the negative one, by virtue of (6), we conclude that (8a) may be equivalently written as an integral over negative E .

$$\int_{-\infty}^0 dE [2\rho_E^s(x) - 2\rho_E^v(x)] + \psi_0^*(x)\psi_0(x) = 0 \quad (8b)$$

Rearranging terms give

$$Q = \int dx \int_{-\infty}^0 dE [\rho_E^s(x) - \rho_0^v(x)] = -\frac{1}{2} \int dx \psi_0(x)\psi_0(x) = -\frac{1}{2}. \quad (9)$$

This is the final result: the soliton's charge is $-\frac{1}{2}$; a fact that follows from completeness (7) and conjugation symmetry (6). It is seen in (9) that the zero-energy mode is essential to the conclusion. The existence of the zero mode in the conjugation symmetric case is assured by the non-trivial topology of the background field. The result is otherwise completely general.

4. The Polyacetylene Story (Quantum Field Theory)

The quantum mechanical derivation that I just presented does not address the question of whether the fractional half-integer charge is merely an uninteresting expectation value or whether it is an eigenvalue. To settle this, we need a quantum field theory approach, that is we need to second quantize the field. For this, we expand Ψ , which now is an anti-commuting quantum field operator, in eigenmodes of our Dirac equation in the soliton sector as

$$\begin{aligned} \Psi &= \sum_{-E}^E (b_E \psi_E^s + d_E^\dagger \psi_{-E}^s) + a\psi_0 \\ \Psi^\dagger &= \sum_{-E}^E (b_E^\dagger \psi_E^{s*} + d_E \psi_{-E}^{s*}) + a^\dagger\psi_0. \end{aligned} \quad (10)$$

The important point is that while the finite energy modes $\psi_{\pm E}^s$ enter with annihilation particle (conduction band) operators b_E and creation anti-particle (valence band) operators d_E^\dagger , the zero mode does not have a partner

and is present in the sum simply with the operator a . The zero energy state is therefore doubly degenerate. It can be empty $| - \rangle$, or filled $| + \rangle$, and the a, a^\dagger operators are realized as

$$a | + \rangle = | - \rangle, \quad a^\dagger | + \rangle = 0, \quad a | - \rangle = 0, \quad a^\dagger | - \rangle = | + \rangle. \quad (11)$$

The charge operator $Q = \int dx \psi^\dagger \psi$ must be properly defined to avoid infinities. This is done, according to Schwinger's prescription in the vacuum sector, by replacing the formal expression by

$$Q = \frac{1}{2} \int dx (\psi^\dagger \psi - \psi \psi^\dagger). \quad (12)$$

We adopt the same regularization prescription for the soliton sector and insert our expansion (10) into (12). We find with the help of the orthonormality of wave functions

$$\begin{aligned} Q &= \frac{1}{2} \sum_E (b_E^\dagger b_E + d_E d_E^\dagger - b_E b_E^\dagger - d_E^\dagger d_E) + \frac{1}{2} (a^\dagger a - a a^\dagger) \\ &= \sum_E (b_E^\dagger b_E - d_E^\dagger d_E) + a^\dagger a - \frac{1}{2}. \end{aligned} \quad (13)$$

Therefore the eigenvalues for Q are

$$Q | - \rangle = -\frac{1}{2} | - \rangle, \quad Q | + \rangle = \frac{1}{2} | + \rangle! \quad (14)$$

5. Conclusion

This then concludes my polyacetylene story, which has experimental realization and confirmation. And the remarkable effect arises from the non-trivial topology of the phonon field in the soliton sector.

Many other topological effects have been found in the field theoretic descriptions of condensed matter and particle physics. Yet we must notice that mostly these arise in phenomenological descriptions, not in the fundamental theory. In condensed matter the fundamental equation is the many-body Schrödinger equation with Coulomb interactions. This does not show any interesting topological structure. Only when it is replaced by effective, phenomenological equations do topological considerations become relevant for the effective description. Fundamental (condensed matter) Nature is simple!

Similarly in particle physics, our phenomenological, effective theories, like the Skyrme model, enjoy a rich topological structure. Moreover, even the Yang-Mills theory of our fundamental "standard particle physics model"

supports non-trivial topological structure, which leads to the QCD vacuum angle. In view of my previous observation, can we take this as indirect evidence that this Yang-Mills based theory also is a phenomenological, effective description and at a more fundamental level – yet to be discovered – we shall find a simpler description that does not have any elaborate mathematical structure. Perhaps in this final theory Nature will be described by simple counting rules – like my first polyacetylene story. Surely this will not be the behemoth of string theory.

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References

1. This research was performed in collaboration with C. Rebbi, and independently by W.P. Su, J.R. Schrieffer and A. Heeger. For a summary see R. Jackiw and J.R. Schrieffer “Solitons with Fermion number $1/2$ in Condensed Matter and Relativistic Field Theories” *Nucl. Phys.* **B190**, 253 (1981).