Fractional Charge from Topology in Polyacetylene and Graphene*

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Abstract

We review the old story of charge fractionalization in polyacetylene, and its newer realization in graphene.

1 Introduction

Discussions of spatial forms for 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 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 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.

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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, with physical consequences for direct meson decays and fermion decay through tunneling.

Here I shall not describe the Yang-Mills investigations; rather I shall show how topological effects in condensed matter situations lead to charge fractionalization. This phenomenon has a physical realization in 1-dimensional (lineal) polymers, like polyacetylene, and in 2-dimensional (planar) systems, like graphene.

The polyacetylene story is old [1]; fractional charge in graphene has been discussed only recently [2]. I shall first sketch the simpler behavior of polyacetylene, and then describe the newer, similar but more complicated graphene story.

2 Polyacetylene Story

Polyacetylene is a material consisting of parallel chains of 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 atoms is about 1Å.

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.

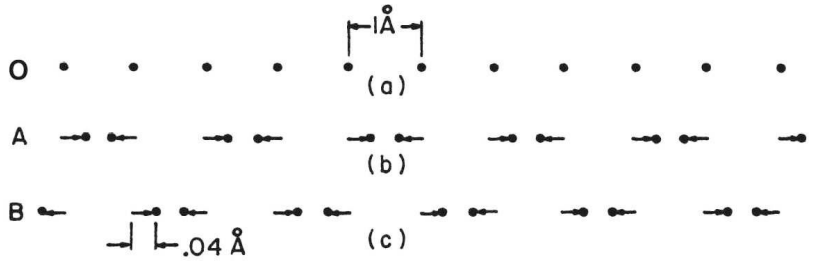

Figure 1: (a) The rigid lattice of polyacetylene; (O) the atoms are equally spaced 1 Å apart. (b), (c) The effect of Peierls' instability is to shift the atoms .04 Å to the right (A) or to the left (B), thus giving rise to a double degeneracy.

It might be thought that these effects merely give rise to a slight fuzzing of the undistorted-lattice situation. In fact this is not so; something more dramatic takes place. Rather 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 ground states, called A and B, see Fig. 1.

If the displacement is described by a real scalar 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, as in Fig. 2. The symmetric point $\phi = 0$ is unstable; the system in

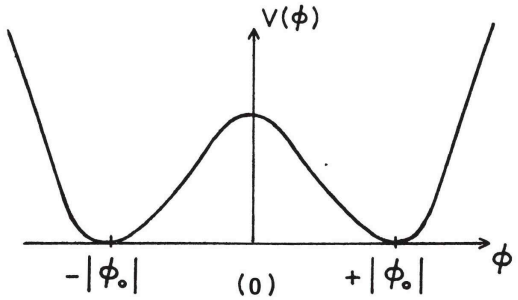

Figure 2: Energy density $V(\phi)$, as a function of a constant phonon field ϕ. The symmetric stationary point, $\phi = 0$, is unstable. Stable vacua are at $\phi = +|\phi_0|$, (A) and $\phi =$ -$|\phi_0|$, (B).

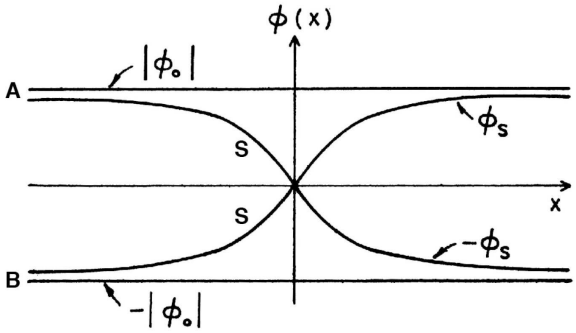

Figure 3: The two constant fields, $\pm \mid \phi_0 \mid$, correspond to the two vacua (A and B). The two kink fields, $\pm\phi_s$, interpolate between the vacua and represent domain walls.

its ground state must choose one of the two equivalent ground states $\phi = \pm \mid \phi_0 \mid = \pm .04$Å. In the ground states, the phonon field has uniform values, independent of x, and leads to a gap (effective mass) in the electron excitation spectrum.

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; see Fig. 3. 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, as in Fig. 4.

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 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 fractionalization [1].

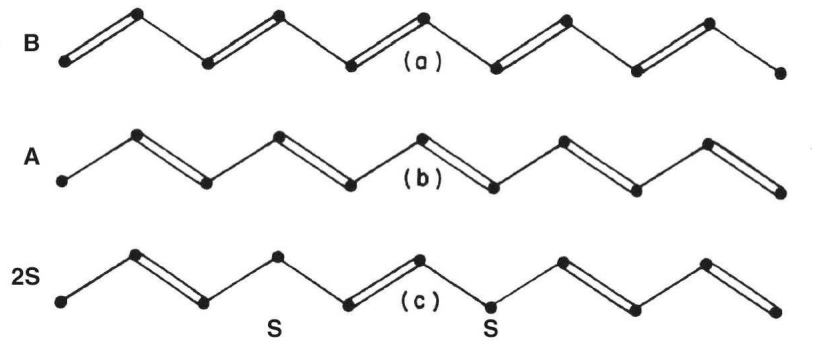

Figure 4: (a), (b) Pattern of chemical bonds in vacua B and A. (c) Two solitons inserted into vacuum A.

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. There 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 fractionalization is without fluctuations; in the limit of infinitely separated solitons one achieves an eigenstate with fractional eigenvalues.

In this simple counting argument no mention is made of topology. The connection to this mathematical concept emerges only when an analytic description is constructed. I now turn to this.

The calculation, which shows how fractional charge arises in the quantum mechanics of fermions interacting with solitons, begins with the observation that fermion motion can be described by a Dirac-like matrix equation. This equation does not arise from relativistic considerations, but rather by linearizing the energy dispersion near the "Dirac points" (intersections of the energy dispersion with the Fermi level). Moreover a distortion of the underlying lattice (Peierls' instability) perturbs the electron motion and couples with strength g the two Dirac points to the lattice distortion — that is, to the phonon field — and to each other. The Dirac equation is in one spatial dimension and involves two components, corresponding to two Dirac points: $h(\phi)\,\psi = (\alpha\, p + g\,\beta\,\phi)\,\psi = E\,\psi,\ \alpha \equiv \sigma^3, \beta \equiv \sigma^2, p \equiv \frac{1}{i}\frac{d}{dx}$. The phonon field satifies the equation $\frac{d^2}{dx^2}\ \phi(x) = V'(\phi(x))$, where V is the double well potential of Fig. 2.

Note that σ^1 anti-commits with the matrices in the Dirac Hamiltonian. Therefore if ψ_E is an eigenfunction with eigenvalue $E, \sigma^1\,\psi_E$ carries eigenvalue $-E$ and an isolated mode must correspond to zero eigenvalue. The positive energy solutions correspond to conduction-band electrons; the negative energy states comprise the valence band and are taken to be filled in the ground state. Here is a schematic summary of the dynamics.

$$H_F = \underbrace{\psi^\dagger\,\alpha\,p\,\psi} + \underbrace{g\,\phi\,\psi^\dagger\,\beta\,\psi}$$

linearization at Fermi level

Peierls' instability

ϕ constant $\phi_0 \Rightarrow$ mass $\mid g\phi_0 \mid$

ϕ soliton $\phi_s \Rightarrow$ zero mode ϕ_0

$$\alpha \equiv \sigma^3, \qquad \beta \equiv \sigma^2, \qquad p = \tfrac{1}{i}\tfrac{d}{dx}$$

$$\sigma'' = V^1(\phi),\ h(\phi)\,\psi = (\alpha\, p + g\beta\,\phi)\,\psi = E\psi$$

A homogenous value for the phonon field gives rise to an effective mass (a gap), while the soliton profile supports an isolated, localized mid gap state — a zero eigenvalue bound state solution to the effective Dirac equation. The isolated mid-gap state is an eigenstate of σ^1. It carries electron number $+1/2$ when filled, $-1/2$ when empty. I shall show how this comes about in the similar, but more complicated context of graphene.

3 Graphene Story

Graphene is a 2-dimensional honeycomb array of atoms forming a hexagonal lattice, which may be viewed as a superposition of two triangular sublattices, **A** and **B**, each possessing two Dirac points; see Fig. 5. So the effective Dirac equation involves four components

(even though the minimal realization of a planar Dirac algebra uses only two components). Again, a lattice distortion (Kekulé distortion) couples the Dirac points to an effective

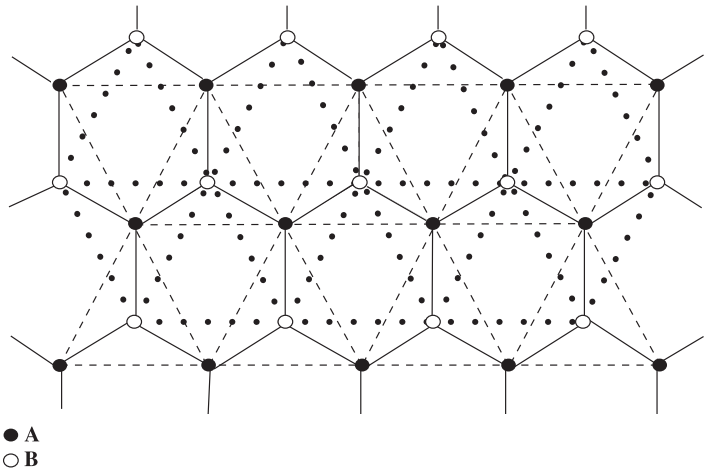

Figure 5: Graphene hexagonal lattice constructed as a superposition of two triangular lattices **A** and **B**.

complex scalar field $\varphi = \varphi_{Re} + i\,\varphi_{Im}$, whose constant value produces a gap.

$$H_0 = \underbrace{\psi^\dagger\, \boldsymbol{\alpha}\cdot\mathbf{p}\,\psi}_{\text{linearization}} + \underbrace{g\,\psi^\dagger\beta\,[\varphi_{Re} - i\,\varphi_{Im}\,\gamma_5]}_{\text{Kekulé distortion}}\ \psi$$

at Fermi level $\qquad\qquad$ φ constant $\varphi_0 \Rightarrow$ mass $\mid g\varphi_0 \mid$

$$\boldsymbol{\alpha} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & -\boldsymbol{\sigma} \end{pmatrix}, \qquad \beta = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \gamma_5 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad \mathbf{p} = \frac{1}{i}\boldsymbol{\nabla}$$

(All vectors are 2-dimensional)

The resulting binding pattern is presented in Fig. 6. The single-double bond alteration is "perfectly matched", in the sense that at each node two single bonds meet one double bond.

Now we enquire whether a soliton profile for φ produces further interesting effects. The natural soliton in two spatial dimensions,where the above theory resides, is a vortex of the Nielsen, Oleson/Landau, Ginsburg, Abrikosov variety. But a vortex also involves a gauge potential **A**, which is not present in H_0. Hence we examine the gauge transformation properties of the theory, with an eye to inserting a gauge potential into the theory. First, there is a global gauge invariance of the fermions, $\psi \to e^{i\chi}\,\psi$, under which the scalar field

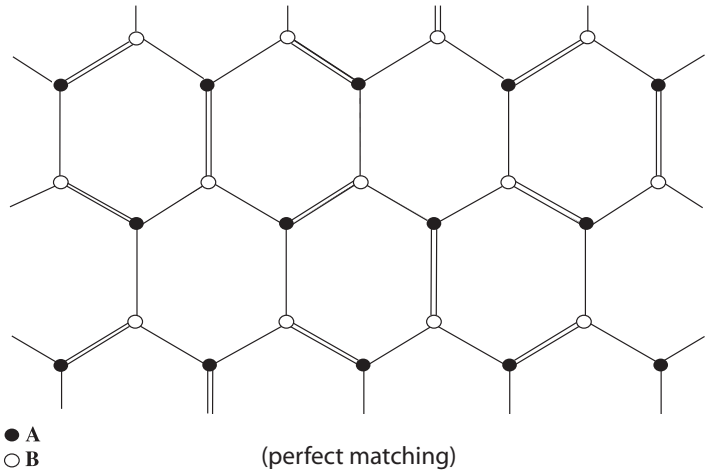

Figure 6: Effect of Kekulé distortion: atoms are closer together for double bonds, further apart for single bonds. The pattern is "perfectly matched": at each node there are two single bonds and one double bond.

φ is neutral. Additionally, the interaction term is invariant against a simultaneous phase change of ψ and φ:

$$\psi \to e^{i\omega\gamma_5}\,\psi, \quad \varphi \to e^{2i\omega}\,\varphi.$$

This invariance may be promoted to a local gauge invariance, provided the kinetic term is gauged by the vector potential $\mathbf{A}$, coupling to ψ in a chiral manner. Thus the complete fermion Hamiltonian becomes [2]

$$H_F = \psi^\dagger \boldsymbol{\alpha}\cdot\left[\mathbf{p} - \gamma_5\,\mathbf{A}\right]\,\psi + g\,\psi^\dagger\,\beta\left[\varphi_{Re} - i\,\gamma_5\,\varphi_{Im}\right]\,\psi,$$

leading to the Dirac equation

$$h(\varphi,\mathbf{A})\,\psi = \boldsymbol{\alpha}\cdot(\mathbf{p} - \gamma_5\,\mathbf{A})\,\psi + g\beta\,(\varphi_{Re}\; - i\,\gamma_5\,\varphi_{Im})\,\psi = E\,\psi.$$

The Bose fields satisfy the vortex equations.

$$\mathbf{D}\cdot\mathbf{D}\,\varphi = \varphi V'\,(\varphi^*\,\varphi)$$

$$\mathbf{D}\,\varphi \equiv (\nabla - i\,2\mathbf{A})\;\varphi$$

$$\frac{1}{e^2}\;\varepsilon^{ij}\,\partial_j\,B = j^i_{\rm BOSE}$$

$$B \equiv \varepsilon^{ij}\,\partial_i\,A^j$$

$$\mathbf{j}_{\rm BOSE} = 4\,Im\,\varphi^*\,\mathbf{D}\,\varphi$$

Here e is a further coupling constant and V is chosen so that at minimum $V' = 0$, $\varphi^* \varphi = \varphi_0^2$, which gives ψ the Dirac mass $\propto |\varphi_0|$. Furthermore, vortex solutions to these equations also exist. Their form is

$$\varphi_v(\mathbf{r}) = \varphi(r)\, e^{in\theta},$$
$$A_v^i(\mathbf{r}) = -n\,\varepsilon^{ij}\,\frac{r^j}{r^2}\; a(r),$$

where n is an integer, $\varphi(r)$ vanishes with r as $r^{|n|}$ and tends to its vacuum value φ_0 at infinity; $a(r)$ vanishes at the origin and tends to $1/2$ at large r. All this ensures finitenes of the vortex energy $E_v = \int d^2 r \left(\frac{1}{2e^2}\; B^2 + \mid \mathbf{D}\varphi \mid^2 + V(\varphi^* \varphi)\right)$. In spite of the presence of the γ_5 matrix, the theory is parity and time-reversal invariant.

Note that α^3 anti-commutes with the matrices in our Dirac Hamiltonian. Therefore if ψ_E is an eigenfunction with eigenvalue E, $\alpha^3\,\psi_E$ belongs to eigenvalue $-E$, and zero modes are eigenstates of α^3. Correspondingly, an unpaired, isolated mode must carry vanishing energy and lie at mid gap. It is easy to verify that indeed such single modes exist at $|n| = 1$.

The total energy for our system is

$$\text{Energy} = E_v + \int d^2 r H_F.$$

Variation of the above Energy with respect to the Fermi field in H_F produces the zero eigenvalue Dirac equation; variation with respect to the Bose fields, produces the vortex equations, but with a back reaction from the coupling to the fermions: $\psi^\dagger \beta\; (1 + \gamma_5)\,\psi$ in the scalar equation, $\psi^\dagger\, \boldsymbol{\alpha}\, \boldsymbol{\gamma}_5\, \psi$ in the gauge field equation. However, with a zero mode that is an eigenstate of α^3, the back-reaction fermion bilinears vanish. Thus our Dirac zero mode, together with the bosonic vortex, provide a self consistent solution to the coupled equations.

Finally we demonstrate that a single mid gap state signals fractionalization of the fermion charge, associated with the global gauge symmetry generated by χ and involving the fermion bilinear $\psi^\dagger\,\psi$ as the charge density. [The charge associated with the local gauge symmetry, generated by ω, includes a contribution from the boson field φ, and does not fractionalize.]

In the ground state all the negative energy Dirac states are filled, so the ground state charge density is constructed from all the negative energy wave functions.

$$\rho(\mathbf{r}) = \int_{-\infty}^{0} d\,E\,\rho_E(\mathbf{r})$$
$$\rho_E(\mathbf{r}) = \psi_E^\dagger(\mathbf{r})\,\psi_E(\mathbf{r})$$

The total charge involves intergrating over $\mathbf{r}$, but this produces an infinity. To renormalize, we measure all charges relative to the ground state in the non-solitonic "vacuum" sector, where the background $\mathbf{A}$ vanishes and φ is a gap producing constant.

The renormalized charge in the soliton/vortex sector then reads

$$Q = \int d^2\, r \int_{-\infty}^{0} d\, E \left(\rho_E^s \left(\mathbf{r}\right) - \rho_E^v \left(\mathbf{r}\right)\right).$$

where the local charge densities $\rho_E(\mathbf{r})$ are constructed from the vacuum Dirac eigenfunction $\psi_E^v \left(\mathbf{r}\right)$ for $\rho_E^v \left(\mathbf{r}\right)$, and from the soliton/vortex eigenfunction $\psi_E^s \left(\mathbf{r}\right)$ for $\rho_E^s \left(\mathbf{r}\right)$. Because of the eigenvalue reflection property, it is also true that $\alpha^3 \, \psi_E = \psi_{-E}$ and therefore $\rho_E = \rho_{-E}$

We are now ready to evaluate Q. Completeness

$$\int_{-\infty}^{\infty} d\, E \, \psi_E \left(\mathbf{r}\right) \psi_E^\dagger \left(\mathbf{r}'\right) = \delta(\mathbf{r} - \mathbf{r}')$$

implies that

$$\int_{-\infty}^{\infty} d\, E \left[\rho_E^s \left(\mathbf{r}\right) - \rho_E^v(\mathbf{r})\right] = 0.$$

In the above integral, we record separately the negative energy contributions; the positive energy contributions, equal to the negative energy contributions because of the eigenvalue reflection property; and finally in the soliton/vortex sector, the zero mode.

$$\int_{-\infty}^{0} dE \, \left\{2[\rho_E^s \left(\mathbf{r}\right) - \rho_E^v \left(\mathbf{r}\right)] + \psi_0^\dagger \left(\mathbf{r}\right) \psi_0 \left(\mathbf{r}\right)\right\}$$

Rearranging and integrating over space gives

$$Q = -\frac{1}{2} \int d^2 r \psi_0^\dagger(\mathbf{r}) \, \psi_0(\mathbf{r}) = -\frac{1}{2}$$

since ψ_0 is normalized.

This then establishes our result; here the argument is presented for 2-dimensional graphene. The same argument, with dimensionality reduced to one, works for polyacetylene.

4 Quantum Field Theory Description

I have established charge fractionalization first by a simple counting argument, then by an argument employing quantum mechanical equations. To finish, I shall use quantum field theory to rederive the result.

We take the Dirac field to be an anti-commuting quantum field operator Ψ. Ψ is expanded in eigenmodes of our Dirac equation in the soliton sector as

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

The important point is that while the finite energy modes $\psi^s_{\pm E}$ enter with annihilation particle (conduction band) operators b_E and creation anti-particle (valence band) operators $d^\dagger_E$, 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 $|->$, or filled $|+>$, and the $a, a^\dagger$ operators act as

$$a\,|+>=|->,\ a^\dagger\,|+>=0,\ a\,|->=0,\ a^\dagger\,|+>=|+>\ .$$

The charge operator $Q = \int d^2r\,\Psi^\dagger\Psi$ 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

$$Q = \frac{1}{2}\int d^2r\,(\Psi^\dagger\Psi - \Psi\Psi^\dagger)\,.$$

We adopt the same regularization prescription for the soliton sector and insert the field expansion into the regularized formula for Q. We find with the help of the orthonormality of wave functions

$$\begin{aligned} Q &= \frac{1}{2}\sum_E (b^\dagger_E\,b_E + d_E\,d^\dagger_E - b_E\,b^\dagger_E - d^\dagger_E\,d_E) + \frac{1}{2}(a^\dagger a - aa^\dagger) \\ &= \sum_E (b^\dagger_E\,b_E - d^\dagger_E\,d_E) + a^\dagger a - \frac{1}{2} \end{aligned}$$

Therefore the eigenvalues for Q are

$$Q\,|->=-\frac{1}{2}|->,\quad Q\,|+>=\frac{1}{2}|+>\,!$$

and the fraction is indeed an eigenvalue.

5 Conclusion

While "Topology" occurs in the title of my talk, no explicit reference was made to topological behavior. The simplicity of the models permitted explicit analysis. However, even without explicit solutions to the relevant equations, one can be assured of the existence of zero modes, thanks to various index theorems that relate such zero modes to the geometry and topology of the backgrounds in which the Dirac equation is solved.

Topology is relevant only to effective, phenomenological descriptions in condensed matter, whose fundamental equation is the many body Schrödinger equation with Coulomb interaction. In particle physics, phenomenological theories like the Skyrme model enjoy a rich topological structure. But also our fundamental Yang-Mills theory has topological effects (QCD vacuum angle, etc.) Does this mean that Yang-Mills theory is phenomenological?

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