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EFFECTS OF DIRAC'S NEGATIVE ENERGY SEA ON QUANTUM NUMBERS

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Quantum physics has taught us that a physical observable need not be a quantity with arbitrary magnitude. Because it is the eigenvalue of a linear Hermitian operator, it will in general be quantized. This is not the case in classical physics, where most observables, like angular momentum and energy are continuously varying so that any value is attainable for them. On the other hand, even in classical physics, there are concepts that are intrinsically integral – for example particle number of conserved particles – and one expects that the integrality will be preserved in the quantum theory, *i.e.*, eigenvalues of the relevant operator – the number operator in our example – are expected to be integers. Quantization of eigenvalues is most easily attained when the operator is a generator of a compact, non-Abelian group, like angular momentum generating $SO(3)$ rotations. However, the number operator frequently generates only Abelian transformations with no group theoretic quantization.

Closer examination of the number operator in a theory with second quantized fermions raises doubts that it will in fact possess only integer eigenvalues. The problem derives from Dirac's negative energy sea, which must be filled to define the vacuum. This involves an infinite number of "particles". Since the number of any further particles must be measured relative to this infinity, there may very well emerge a non-integral answer. Nevertheless, it has been believed that various renormalization procedures, like normal ordering, can unambiguously insure integrality of the eigenvalue. Therefore, it was a suprise when it was established about a decade ago[1] that fermions moving in the field of a topologically non-trivial soliton (kink in one spatial dimension, vortex in two, monopole in three) possess non-integer eigenvalues for their number operator. It is perhaps even more surprising that this peculiar effect has a physical realization in properties of actual condensed matter systems – polyactylene being the standard example.[2] Here, I shall describe this to you, first in a general, formal way, and then in a physically intuitive language appropriate to polyacetylene.

We wish to second quantize fermions moving in a static background which generically is described by φ. Fermion dynamics is governed by a Dirac Hamiltonian $H(\varphi)$. Two different backgrounds are envisioned: one is appropriate for the vacuum sector of the theory φ_v, the other for the soliton φ_s. For example, φ may be a condensate field which takes a homogenous value in the vacuum sector and a topologically non-trivial profile in the soliton sector.

Second quantization proceeds by computing the energy eigenvalues and eigenfunctions of $H(\varphi)$, which possesses both positive and negative energy eigenstates, and "filling" the

negative energy sea. The number density of the soliton ground state is given by

$$\rho(\mathbf{x}) = \sum\!\!\!\!\!\!\int_{-\infty}^{0^-} dE \left(|\Psi_E(\mathbf{x})|^2 - |\psi_E(\mathbf{x})|^2\right) \tag{1}$$

where the integration, which also includes summutation over discrete levels, extends over all negative energy states, since they are filled in the vacuum. Here Ψ_E is the energy eigenfunction in the presence of the soliton and ψ_E is the eigenfunction in the vacuum sector.

$$H(\varphi_s)\Psi_E = E\Psi_E, \quad H(\varphi_v)\psi_E = E\psi_E \tag{2}$$

The fermion number of the soliton vacuum is the spatial integral of ρ.

$$N_F = \int d\mathbf{x}\ \rho(\mathbf{x}) \tag{3}$$

It is a very beautiful aspect of the theory that one can evaluate (1) and (3) by general mathematical methods, which bypass solving the eigenvalue problem (2) explicitly. Rather, one uses spectral sum rules whose form is dictated by general features of the Hamiltonian, in particular by the topological properties of the background φ and of the space $\{\mathbf{x}\}$.[3] While these methods are powerful, they are also technical, requiring much mathematical knowledge; so I cannot present them here. However, when the Hamiltonian posseses one further property, the sum rules become trivial, and the result for N_F is immediate.

We assume further that $H(\varphi)$ possesses a conjugation symmetry which takes positive energy states into negative energy states and *vice versa*; *i.e.*, we assume there exists an operator C which anti-commutes with $H(\varphi)$: $C^{-1}HC = -H$. One consequence of this is that the number density at E is an even function of E: $|\Psi_E|^2 = |\Psi_{-E}|^2$, $|\psi_E|^2 = |\psi_{-E}|^2$. A less obvious consequence is that in the soliton sector, there are always normalizable, discrete zero-energy modes.

$$H(\varphi_s)u_0 = 0, \quad \int d\mathbf{x}|u_0(\mathbf{x})|^2 = 1 \tag{4}$$

This fact may be seen by explicit solution of the eigenvalue problem, but it also follows from a general mathematical argument, called *index theory*, which insures that the Dirac operator has normalizable zero-energy modes in the presence of a topologically non-trivial background.[3]

We are now in a position to evaluate (1) and (3). First, we use completeness of the eigenfunctions in the soliton and vacuum sectors.

$$\sum\!\!\!\!\!\!\int_{-\infty}^{0^-} dE|\Psi_E(x)|^2 + \sum\!\!\!\!\!\!\int_{0^+}^{\infty} dE|\Psi_E(\mathbf{x})|^2 + |u_0(\mathbf{x})|^2 - \sum\!\!\!\!\!\!\int_{-\infty}^{\infty} dE\ |\psi_E(\mathbf{x})|^2 = 0 \tag{5}$$

The zero-energy mode in the soliton sector has been explicitly separated; we assume there is just one. (In the vacuum sector there are none.) Then, use of the conjugation symmetry allows equating the positive energy integrals with the negative energy ones, and converts (5) into an evaluation of (1).

$$\not\int_{-\infty}^{0^-} dE \ \left(|\Psi_E(\mathbf{x})|^2 - |\psi_E(\mathbf{x})|^2\right) = -\frac{1}{2}|u_0(\mathbf{x})|^2 \tag{6}$$

The spatial integration which determines N_F is trivial since the zero mode is normalized.

$$N_F = -\frac{1}{2} \tag{7}$$

The conclusion is that the soliton vacuum, defined with the zero mode empty, carries fermion number $-\frac{1}{2}$; of course, when the zero mode is filled, this fermion number is $+\frac{1}{2}$! The fermion number assignment of $\pm\frac{1}{2}$ for two states degenerate in energy is the only possible one consistent with a conjugation-odd fermion number operator.

Several comments should be made in connection with this very elementary derivation of our surprising result.

(i) The above evaluation concerns the *expected* value of the second-quantized, field theoretic number operator, $\hat{N}_F$. However, one can easily show, by expanding the second quantized field in terms of creation and annihilation operators in the presence of the soliton,[1] that in fact the *eigenvalues* are $\pm\frac{1}{2}$.

(ii) A useful way for thinking about the effect is in terms of vacuum polarization:[4] The soliton polarizes the normal vacuum and produces the fractional quantum number, by distoring the negative energy sea.

(iii) We have viewed the soliton as an external field. In a complete description, one must take the soliton's quantum dynamics into account. Necessarily there will occur spontaneous symmetry breaking in the vacuum sector. Calculations in the full theory can be carried out by Monte-Carlo methods, or by analytic techniques of the Born-Oppenheimer variety.

The three ingredients necessary for fermion number fractionization – spontaneous symmetry breaking, solitons and fermions – come together in a description of a physical system, polyacetylene. This is a one-dimensional array of carbon atoms which can form one of two degenerate ground states. The degeneracy arises from a spontaneous breaking of the right-left symmetry (Peierls instability) and manifests itself in an alteration of the bonding pattern, as illustrated in Fig. 1.

A microscopic Hamiltonian for the system has been proposed by Su, Schrieffer and Heeger (SSH).[2] In the continuum and infinite volume limit, electron transport is governed

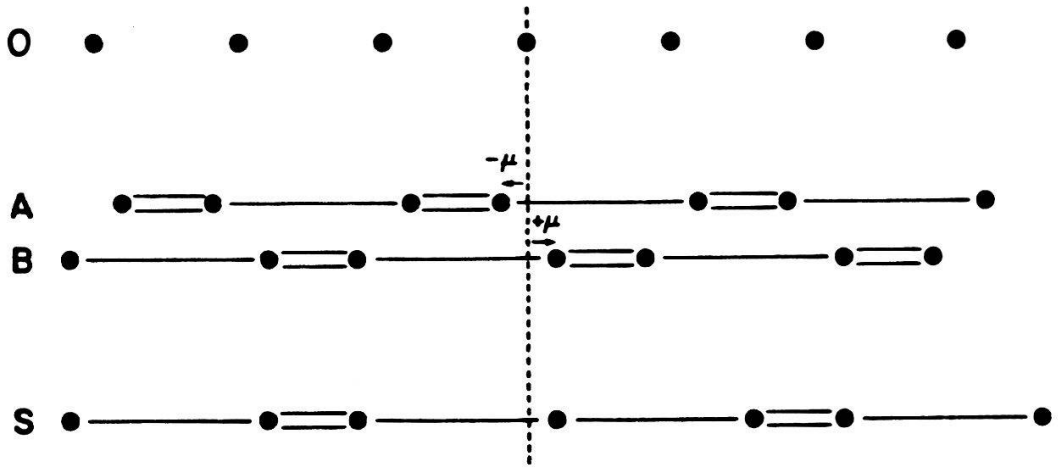

Fig. 1: Polyacetylene consists of a linear chain of carbon atoms (dots). The equally spaced configuration (O) possesses a left-right symmetry, which however is energetically unstable. Rather in the ground states the carbon atoms shift a distance μ to the left or right, breaking the symmetry and producing two degenerate ground states (A, B). (The drawing is not to scale; the shift is only a few percent of the total bond length.) A soliton (S) is a defect in the alteration patters; it provides a domain wall between configurations (A) and (B).

by a Dirac-type Hamiltonian in one dimension.[5]

$$H(\varphi) = \sigma_3 \hat{p} + \sigma_1 \varphi(x), \quad \hat{p} = \frac{1}{i}\frac{d}{dx}$$
$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{8}$$

Here, $\varphi(x)$ is the phonon field; it measures the displacement of the carbon atom from its equalibrium position. The matrix structure of the above Hamiltonian does not arise from spin. In the SSH description, electron-electron interactions are ignored and spin is a passive label; the Hamiltonian in (8) describes separately spin up and spin down electrons. Rather, the two-component wavefunctions which are eigenmodes of (8) refer to the right-moving and left-moving electrons with momentum $\pm|p|$. The filled negative energy states of H are the valence electrons, while the conduction electrons populate the positive energy states.

In the SSH model, $\varphi(x)$ is determined self-consistently by the phonon's dynamics, and in the lowest (vacuum) states $\varphi(x)$ takes the uniform values $\pm\mu$, as illustrated in Fig. 1. The corresponding spectrum of (8) exhibits a gap.

In addition to the two ground states, where the phonon field takes a constant value, there exist stable excited states where $\varphi(x)$ assumes a kink shape, which interpolates as x passes from $-\infty$ to $+\infty$, between the vacuum configurations $-\mu$ and $+\mu$. This is the soliton, and it describes a defect in the alteration pattern, as is also exhibited in Fig. 1.

The Hamiltonian in (8) admits a conjugation symmetry: $C = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ anti-commutes with H – this is ordinary charge conjugation invariance in the absence of Coulomb interactions. The zero eigenvalue problem is solved easily with a kink background; there is one normalizable zero-energy solution. Thus, our general analysis predicts that fermion number, here coinciding with charge, fractionizes to $\pm\frac{1}{2}$ in the one-soliton state.

This result may also be seen pictorially. When two solitons are inserted into the ground state (B), the bonding pattern is depicted in Fig. 2. Note that the number of bonds in the two-soliton state is one fewer than in the ground state. If the two solitons are now separated far apart, so that they act independently, the quantum numbers of the missing bond must be shared between the two states, and that is how the fraction $\frac{1}{2}$ arises.

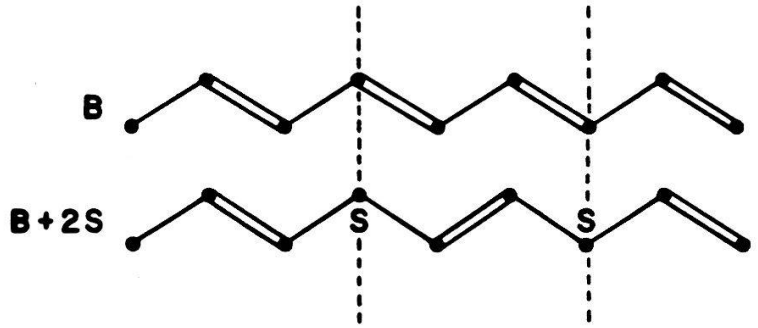

Fig. 2: With two solitons (SS) inserted in vacuum (B), the number of bonds between the sites of the defects decreases from five to four.

I hasten to add that fractional charge has not in fact been observed in experiments on polyacetylene. The reason is that electrons come in two species, spin up and spin down. Since both contribute to the number density, the charge in the unfilled ground state is $-\frac{1}{2}\times 2 = -1$, while the filled state is neutral: $-1+1 = 0$. Nevertheless, charge fractionization leaves a spur: the soliton state with unfilled zero-energy state has net charge, but no net spin since all electron spins are paired. When the level is filled, there is no net charge, but now there is net spin. These spin-charge assignments (charged-without spin, neutral-with spin) are unexpected, but in fact have been observed and provide experimental, to be sure indirect, verification for the soliton picture of polyacetylene.[6]

Moreover, there are systems without a conjugation symmetry.[7,8] For example, replace every other carbon atom in polyacetylene by a different atom. In the approximation that the energy levels of both atoms are the same, except for an overall energy shift 2ϵ, the electron Hamiltonian becomes $H = \sigma_3\hat{p} + \sigma_1\varphi + \epsilon\sigma_2$. No quantity anti-commutes with this and the charge can no longer be computed as simply as above. The answer, obtained by other methods, is[4,8,9]

$$N_F = -\frac{1}{\pi}\tan^{-1}\frac{\mu}{\epsilon} \tag{9}$$

which reduces to $-1/2$ as ϵ vanishes.

Of course, for actual physical samples, where the volume and the separation between defects are finite, the non-integer fermion number is only an expectation value for the operator $\hat{N}_F$, and there are corrections which vanish in the infinite limit. The important point is that the variance $\langle \hat{N}_F^2 \rangle - \langle \hat{N}_F \rangle^2$ also vanishes in the limit.[10] This is to be contrasted to the uninteresting situation of, say, an electron circulating about two nuclei. When the nuclei are far apart, the expected value for electron number near each nucleus is $\frac{1}{2}$, plus small corrections. However, the variance remains $\frac{1}{4}$ for infinite separation, which shows that this fraction never becomes an eigenvalue.

The concept of fractional quantum numbers has now extended beyond soliton systems – for example the theory of the quantum Hall effect makes us of the idea, even though its detailed dynamics is quite different from the above examples.[11]

While fractional quantum numbers were first seen in relativistic field theory, thus far they have not played any experimentally verified role in particle physics. Nevertheless, it is curious that an effect which in principle is physical should arise from distortions in the negative energy sea, which for particle physics is an unphysical construct, in contrast to the condensed matter application, where negative energy states correspond to physical quantities – the valence electrons.

However, there is another, physically realized circumstance in particle physics where the Dirac negative energy sea modifies symmetry behavior of fermions. This is the chiral anomaly phenomenon whereby the axial vector currect $i\bar{\psi}\gamma^\mu\gamma^5\psi$, which is conserved for free massless Dirac fermions, ceases to be conserved when the massless fermions interact with a gauge field, even though the interaction is chirally invariant.[12] The problem afflicts only the second quantized theory, and conventionally is associated with infinities that plague relativistic quantum field theory: the infinities must be regulated and renormalized, but there is no chirally invariant regulator procedure. However, a more directly physical discussion of the anomaly phenomenom may be given, which shows that in fact it is the filling of the negative energy sea that breaks the chiral symmetry.[13]

Let me first state the essential puzzle of the chiral anomaly. Consider a massless Dirac fermion moving in a background gauge field A_μ. The dynamics is governed by a Lagrangian which splits into separate right and left parts.

$$\begin{aligned} \mathcal{L} &= \bar{\psi}(i\not{\partial} - e\not{A})\psi \\ &= \bar{\psi}_+(i\not{\partial} - e\not{A})\psi_+ + \bar{\psi}_-(i\not{\partial} - e\not{A})\psi_- \\ \psi &= \psi_+ + \psi_-, \quad \psi_\pm = \frac{1}{2}(1 \pm i\gamma_5)\psi \end{aligned} \tag{10}$$

In the first-quantized theory, where ψ is a wavefunction and $\bar{\psi}\gamma^\mu\psi$ is a probability current, the separate right and left currents are conserved, and the separate probabilities $\int d\mathbf{x}\, \psi_\pm^\dagger \psi_\pm$

are time-independent. In the second quantized theory, where ψ becomes an operator, the anomaly phenomenon renders the separate right and left currents no longer conserved, and the right and left charges are not time-independent. Nevertheless, the sum of right and left currents – the vector current – is conserved, while the divergence of the difference between the right and left currents – the axial vector current – is non-zero owing to the anomaly. Our task then is to understand what causes the separate non-conservation of left and right currents even though there is no coupling between the two apparent in (10).

Evidently, the problem derives from the second quantization procedure, hence we review it. We set A^0 to zero, find the eigenmodes of the Hamiltonian in the background field $\mathbf{A}$, and define the second quantized vacuum by filling the negative energy modes, leaving the positive energy modes empty. The background $\mathbf{A}$ is chosen in a specific functional form so that the anomaly is non-vanishing. This requires a time-dependence for $\mathbf{A}$, but we chose a potential constant in time and space and model the time variation by an adiabatic change $\mathbf{A} \to \mathbf{A} + \delta\mathbf{A}$.

The simplest model to study is two-dimensional and Abelian – two-dimensional massles quantum electrodynamics.[14] The Dirac matrices are 2×2 and ψ is a two-component spinor.

$$\begin{aligned} &\gamma^0 = \sigma^1, \quad \gamma^1 = i\sigma^2, \quad \gamma_5 = i\gamma^0\gamma^1 = -i\sigma^3 \\ &\psi_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\psi, \quad \psi_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\psi \end{aligned} \tag{11}$$

The axial current possess an anomalous divergence proportional to $\epsilon^{\mu\nu}F_{\mu\nu} \propto \partial_t A^1$.[15] The eigenmodes to be second quantized satisfy a one-dimensional Dirac equation,

$$H\psi_E = \alpha(\hat{p} - eA)\psi_E = E\psi_E, \quad \alpha = -\sigma^3 \ , \tag{12}$$

where $A \equiv A^1$ is constant. They are given by

$$\begin{aligned} \psi_+ &= \begin{pmatrix} e^{ipx} \\ 0 \end{pmatrix} \text{ with } E = -p + eA \\ \psi_- &= \begin{pmatrix} 0 \\ e^{ipx} \end{pmatrix} \text{ with } E = p - eA \end{aligned} \tag{13}$$

Second quantization is performed by filling the negative energy sea. For $A = 0$, the energy-momentum dispersion is depicted in Fig. 3, where the right-hand branch corresponds to fermions of one chirality, and the left-hand branch to those of the other chirality. The negative energy states are filled, as indicated by the filled circles; the positive energy states are empty, as indicated by the empty circles. As A increases from 0 to δA, empty states in the right-hand branch acquire negative energy, while filled states of the left-hand branch

become positive energy states; *i.e.*, there is a net production of right-handed antiparticles and left-handed particles; see Fig. 4. So the separate right and left charges are not conserved, but their sum is. Put in another way, the separation between positive and negative energy states of definite chirality cannot be achieved gauge-invariantly, since changing A from 0 to a constant δA is a gauge transformation, yet particles are produced.

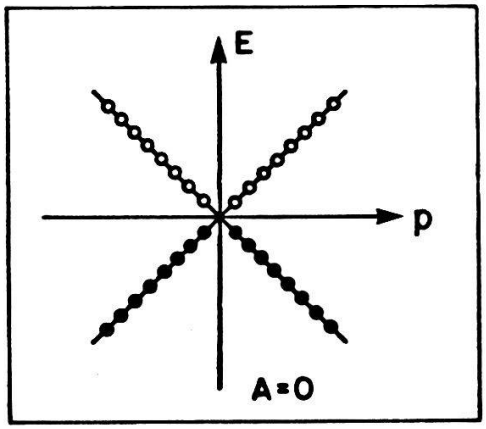

Fig. 3: Energy-momentum dispersion at $A = 0$. Empty circles are empty states; filled circles are filled states.

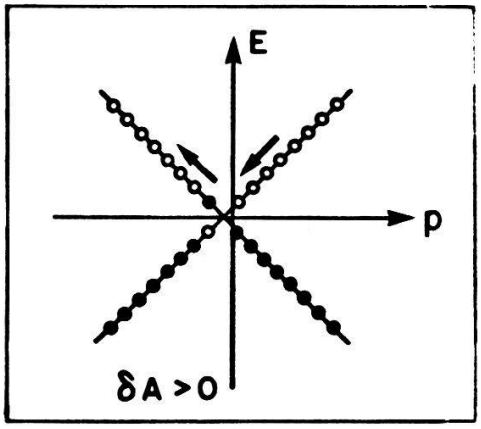

Fig. 4: Energy-momentum dispersion at $A = \delta A > 0$. The energy shift produces negative energy empty states and positive energy filled states.

We thus see that the negative energy sea is responsible for non-conservation of chirality even though the dynamics is chirally invariant. This effect was called *anomalous* because its discovery was an unexpected surprise. However, a better name might be *quantum mechanical symmetry breaking* – a symmetry breaking mechanism which like Heisenberg's *spontaneous symmetry breaking*, attributes physical asymmetry to the vacuum state and not to the dynamics. Here, however, unlike in Heisenberg's case, it is not vacuum degeneracy, but the very definition of the vacuum that is responsible.

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