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Elementary derivation of one-dimensional fermion-number fractionalization

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An elementary explanation of the origin of topological or fractional charges in one dimension is presented. Attention is paid to where the balance of the charge is located and the influence of the choice of boundary conditions on the problem.

I. INTRODUCTION

In a variety of different contexts in both condensed matter physics and relativistic quantum-field theory, a Fermi sea in interaction with a solitonlike external field can endow the soliton with fractional or otherwise unusual quantum numbers. Examples occur in one-dimensional polymers such as polyacetylene,¹ in ³He superfluids,² and in bag³ or Skyrme⁴ models of hadrons. Since the original observation of this effect by Jackiw and Rebbi,⁵ a variety of sophisticated tools have been used to analyze the phenomenon: index theorems and ζ function methods by the more mathematically inclined,⁶ Green's functions,⁷ Jost functions,⁸ and anomalies⁹ by the physicist. The more powerful the tool employed, the deeper the results obtained-but often at the expense of losing a simple physical picture. I am sure that many people have felt uneasy about what is happening until they have worked out simple examples such as those recently published by Mackenzie and Wilczek,¹⁰ and by Zahed.¹¹ My purpose here is to give an elementary proof, using nothing more technical than integration by parts, of the general result that a charge

$$Q = q \frac{\Delta \theta}{2\pi} \tag{1.1}$$

can be locally induced in a one-dimensional Dirac-Hamiltonian for particles of elementary charge q.

II. PHASE-SHIFTS AND LEVINSON THEOREMS

The Hamiltonian which occurs in many of these contexts is

$$H = i\sigma_1 \partial_x + \phi_1(x)\sigma_2 + \phi_2(x)\sigma_3 \quad , \qquad (2.1)$$

where σ_1 are the Pauli matrices. (The interpretation of the two components varies with the context. In polyacetylene they are the odd and even sites. In ³He-A they are particles and holes.) I shall concentrate on the case where ϕ_1, ϕ_2 are asymptotically constant and where, for simplicity, $(\phi_1^2 + \phi_2^2)^{1/2}$ takes the same values on both sides of the region in which ϕ_1, ϕ_2 are varying. The local charge is

$$\rho(x) = q \sum_{\substack{\text{negative} \\ \text{energy} \\ \text{states}}} \psi^{\dagger}(x)\psi(x) , \qquad (2.2)$$

where the ψ are properly normalized two-component spi-

nors. If we define an angle $\theta(x)$ by

$$\frac{\phi_2}{\phi_1} = \tan\theta \quad , \tag{2.3}$$

it is our goal to establish that

$$Q = \int dx \,\rho(x) = q \frac{\Delta\theta}{2\pi} \quad , \tag{2.4}$$

where $\Delta \theta$ is the change in θ as we cross the region of varying θ .

To make the problem well defined we must establish boundary conditions for the differential operator (2.1). Periodic boundary conditions are not suitable since (2.1) is a different equation at the two ends when $\Delta \theta \neq 0$. Let us choose self-adjoint boundary conditions (BC's) at the two ends separately.

Self-adjoint BC's are such that¹²

$$\int_{x_1}^{x_2} dx [\chi^{\dagger} H \psi - (H \chi)^{\dagger} \psi] = i (\chi^{\dagger} \sigma_1 \psi) \Big|_{x_1}^{x_2} = 0 \quad , \qquad (2.5)$$

for all permitted solutions χ, ψ , i.e.,

$$(\chi_1^*\psi_2 + \chi_2^*\psi_1)\big|_{x_1} = 0 \tag{2.6}$$

or

$$\frac{\chi_1}{\chi_2}\Big|_{\mathbf{x}_i} = \frac{\psi_1}{\psi_2}\Big|_{\mathbf{x}_i} = -i \tan\theta_i \quad , \tag{2.7}$$

for some angles θ_1 , θ_2 [not to be confused with $\theta(x)$] defined at the ends x_1 , x_2 .

We will temporarily leave open the choice of these angles as it will turn out that some choices are more convenient than others—although the local effect of the changing $\theta(x)$ is independent of effects at a distant boundary.

We will obtain the induced charge from phase shifts and to do this it helps to have an equation of fixed asymptotic form. To achieve this we use the identity

$$H = \exp[-i\theta(x)\sigma_1/2][i\sigma_1\partial_x + (\phi_1^2 + \phi_2^2)^{1/2}\sigma_2 + \frac{1}{2}\partial_x\theta]$$
$$\times \exp[i\theta(x)\sigma_1/2]$$

 $= \exp[-i\theta(x)\sigma_1/2]H'\exp[+i\theta(x)\sigma_1/2] \quad (2.8)$

If ψ is an eigenfunction of H then

$$\psi' = e^{i\sigma_1 \theta(x)/2} \psi \tag{2.9}$$

is an eigenfunction of H'-provided we change the boun-

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dary angles for H' to $\theta_i' = \theta_i - 1/2\theta(x_i)$. This is because

$$\exp\left(\frac{1}{2}i\theta\sigma_{1}\right)\left(\frac{\sin\theta_{i}}{i\cos\theta_{i}}\right) = \left(\frac{\sin\left(\theta_{i} - \frac{1}{2}\theta\right)}{i\cos\left(\theta_{i} - \frac{1}{2}\theta\right)}\right) \quad . \tag{2.10}$$

It is the θ'_i which is convenient to fix to certain values. The reason for this is that, when $\partial_x \theta = 0$, H' has a symmetry between positive and negative energies induced by the identity

$$\sigma_3 H' = -H' \sigma_3 \quad . \tag{2.11}$$

For the boundary conditions to respect this symmetry we must arrange for ψ' , $\sigma_3\psi'$ to both satisfy the boundary conditions. This requires $\theta'_i = 0, \pi/2$. Further, unless we choose the left-hand (θ_1) value to be 0 and the right-hand value to be $\pi/2$, there will be bound states attached to the ends (see Appendix). We want particle-hole symmetry and no bound states or else there will be locally induced charges near the boundary and this will be confusing. (In the case of a monopole in a θ vacuum the monopole is the boundary and the boundary charge is the physical effect of impor-

tance. This case has been dealt with by $Grossman^{13}$ and $Yamagishi.^8$)

We will now prove a "relativistic" form of Levinson's theorem (otherwise known as the Friedel sum rule) by a simple extension of a problem in Landau and Lifshitz.¹⁴⁻¹⁶ Let us rewrite H' as

$$H' = i\sigma_1 \partial_x + m(x)\sigma_2 + V(x) \quad , \tag{2.12}$$

where

$$m(x) = (\phi_1^2 + \phi_2^2)^{1/2} \to m \text{ as } x \to \infty ,$$

$$V(x) = \frac{1}{2} \partial_x \theta \to 0 \text{ as } x \to \infty .$$

Let us also set $x_1 = 0$.

At large distances (2.12) has solutions of the form

$$\psi_{k}^{(\pm)}(x) = \begin{bmatrix} 1\\ i\frac{(\partial + m)}{E_{k}^{(\pm)}} \end{bmatrix} \sin(kx + \delta_{\pm}) ,$$

$$E_{k}^{(\pm)} = \pm (k^{2} + m^{2})^{1/2}, \quad k > 0 .$$
(2.13)

Now

$$\int_{0}^{R} \left[\left(\psi_{k'}^{(\pm)} \right)^{\dagger} H' \psi_{k}^{(\pm)} - \left(H' \psi_{k'}^{(\pm)} \right)^{\dagger} \psi_{k'}^{(\pm)} \right] dx = \left(E_{k}^{(\pm)} - E_{k'}^{(\pm)} \right) \int_{0}^{R} \left(\psi_{k'}^{(\pm)} \right)^{\dagger} \psi_{k}^{(\pm)} dx = \left[\left(\psi_{k'}^{(\pm)} \right)^{\dagger} i \sigma_{1} \psi_{k}^{(\pm)} \right]_{0}^{R}$$
(2.14)

Put k' + dk = k and substitute the form (2.13). After a little arithmetic we find

$$\frac{\partial E^{(\pm)}}{\partial k} \int_{0}^{R} |\psi_{k}^{(\pm)}|^{2} dx = \frac{1}{E^{2}} \frac{\partial E^{(\pm)}}{\partial k} \sin(kR + \delta_{\pm}) [(\partial_{x} + m) \sin(kx + \delta_{\pm})]_{x=R} + \left(R + \frac{\partial \delta_{\pm}}{\partial k}\right) \frac{k}{E^{(\pm)}} - \frac{1}{2E^{(\pm)}} \sin^{2}(kR + \delta_{\pm}) \quad .$$
(2.15)

Using $\partial E^{\pm}/\partial k = k/E^{(\pm)}$ we find

$$\int_0^R |\psi_k^{(\pm)}|^2 dx = \left(R + \frac{\partial\delta\pm}{\partial k}\right) - \frac{1}{2k}\sin^2(kR + \delta\pm) + \frac{1}{E^2}\sin(kR + \delta\pm)[(\partial + m)\sin(kx + \delta\pm)]_{x=R} \quad (2.16)$$

This is our key result as it identifies the extra normalization pulled into the region by the potential V. If $\partial \theta(x) > 0$, positive energy particles are repelled from the potential while negative energy ones are attracted and this is the origin of the local charge.

To use (2.16) we need the values of δ_{\pm} at k=0 and $k=\infty$. These are easily found. For large k H' becomes

$$H' = \begin{pmatrix} V(x) & i\partial_x \\ i\partial_x & V(x) \end{pmatrix} , \qquad (2.17)$$

since we can ignore m compared to k in the off-diagonal elements. Thus

$$\psi_{k}^{\pm}(x) = \begin{bmatrix} \sin\left(Ex - \int_{0}^{x} dx \ V(x)\right) \\ i \cos\left(Ex - \int_{0}^{x} dx \ V(x)\right) \end{bmatrix} , \qquad (2.18)$$

with $E = \pm k$ and where I am using the boundary condition $\theta'_1 = 0$ at x = 0. Comparison with (2.13) reveals that

$$\delta_{+}(k=\infty) = -\int_{0}^{\infty} V(x) dx = -\frac{1}{2}\Delta\theta ,$$

$$\delta_{-}(k=\infty) = +\int_{0}^{\infty} V(x) dx = +\frac{1}{2}\Delta\theta .$$
(2.19)

For k = 0 we notice that if we multiply V by λ then $\partial \delta / \partial \lambda$ gives the flow of eigenvalue density for H' and this must be zero at k = 0 (the edges of the continua) unless a bound state escapes into the gap when δ changes by π . Thus $\delta \pm (0) = n\pi$.

We can now calculate Q by first normal ordering so that Q = 0 if there is particle-hole symmetry:

$$\rho = q \sum_{\substack{\text{negative} \\ \text{energy} \\ \text{states}}} |\psi|^2 - \frac{1}{2}q \sum_{\substack{\text{all} \\ \text{states}}} |\psi|^2 \quad . \tag{2.20}$$

The subtraction term is a V independent of infinity by completeness. Thus

$$\rho(x) = -\frac{q}{2}\eta(x) = -\frac{q}{2}\sum_{\substack{\text{all}\\\text{states}}} \operatorname{sgn}(E)|\psi|^2 \quad (2.21)$$

This local form of the η invariant¹⁷ (or spectral asymmetry) is finite and needs no regularization.

We can perform the continuum parts of the sum by noting that, as long as the system has length L large compared to the support of $\partial\theta$, the normalization integral is $\sim L$ and the density of states $dn/dk \sim L/\pi$. So we obtain the continuum contribution to the charge between 0 and R by multiplying by π^{-1} and integrating over k.

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$$\int_{0}^{\infty} \frac{dk}{\pi} \int_{0}^{R} \{ |\psi_{i}^{(+)}|^{2} - |\psi_{k}^{(-)}|^{2} \} dx = \frac{1}{\pi} [\delta_{+}(\infty) - \delta_{+}(0) - \delta_{-}(\infty) + \delta_{-}(0)] + \text{terms small as } R \to \infty \quad .$$
(2.22)

The smallness of the oscillating terms' contribution to the integral follows from the Rieman-Lebesgue lemma and the vital fact that $\delta(0) = n\pi$ renders the k^{-1} singularity in the second term of (2.16) harmless. Thus

$$\lim_{R \to \infty} \int_{0}^{R} \rho(x) dx = -\frac{1}{2} (N_{p} - N_{n}) + q \frac{\Delta \theta}{2\pi} + \frac{q}{2\pi} [\delta_{+}(0) - \delta_{-}(0)] , \qquad (2.23)$$

where N_p is the number of positive-energy bound states and N_n is the number of negative-energy bound states. Information on the bound states can be found by adding, instead of subtracting the two terms and using completeness: if $\psi_{k,0}^{(\pm)}$ are the solutions of H' with m = constant and V = 0

$$\lim_{R \to \infty} \left[\int_0^R \left(\sum_{\substack{\text{bound} \\ \text{states}}} |\psi|^2 \right) dx + \int_0^\infty \frac{dk}{\pi} \int_0^R \left(|\psi_k^{(+)}|^2 + |\psi_k^{(-)}|^2 - |\psi_{k,0}^{(+)}|^2 - |\psi_{k,0}^{(-)}|^2 \right) dx \right] = 0 = N_B - \frac{1}{\pi} \left[\delta_+(0) + \delta_-(0) \right] \quad , \quad (2.24)$$

where N_B denotes the number of bound states. This agrees with our assertion that the number of bound states escaping from the two continua are $\delta_+(0)/\pi$, $\delta_-(0)/\pi$, respectively. So, up to the number of levels crossing zero—and consequently being counted as filled by the formulae—we have

$$\int \rho(x) dx = q \frac{\Delta \theta}{2\pi}$$

as promised.

III. DISCUSSION

Twisting the BC's at the same time as changing θ is very natural. In most systems the solitons will occur in pairs — one with +Q and one with -Q. Cutting the system between them leaves us with the rotated BC's. Any other choice leaves us with a charge located at the boundary. It is instructive to repeat the calculations with θ_i (not θ'_i) left fixed at zero so $\theta'_1 = -\theta(x_1)/2$. We find that the θ_1 contribution to $\int_0^0 \rho(x) dx$ is canceled by a charge at the boundary x_1 . This means that, of the total charge $q[\theta(x_2) - \theta(x_1)]/\pi$ on the soliton, the $q\theta(x_1)/\pi$ has resulted from charge expelled to the left and $q\theta(x_2)/\pi$ from charge attracted from the right. The total charge has stayed fixed and the expelled charges can be found within a distance m^{-1} of the right- and left-hand boundaries. A brief discussion of these bound states and charges at the system boundaries is included in an Appendix.

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APPENDIX: BOUND STATES AT BOUNDARIES

Near the boundary H' is of the form

$$H' = \begin{bmatrix} 0 & i(\partial - m) \\ i(\partial + m) & 0 \end{bmatrix} .$$
 (A1)

A bound state of the form

$$\psi = \begin{pmatrix} E\\ i(\partial + m) \end{pmatrix} e^{\alpha x} \tag{A2}$$

can exist near the boundary if α has the appropriate sign, $m^2 = E^2 + \alpha^2$, and if ψ satisfies the BC

$$\psi(0) \propto \left(\frac{\sin\theta'}{i\cos\theta'} \right) . \tag{A3}$$

Put $\alpha = m \cos \chi$, $E = m \sin \chi$ then

$$\psi(0) = m \begin{pmatrix} \sin \chi \\ i(1 + \cos \chi) \end{pmatrix} , \qquad (A4)$$

so $\tan\theta' = \tan(\chi/2)$. There is a bound state at the left if $\alpha < 0$, i.e., $\pi/4 < \theta'_1 < 3\pi/4$ and one at the right if $0 < \theta'_2 < \pi/4$, $3\pi/4 < \theta'_2 < \pi$.

Let us concentrate on the left-hand boundary where one can easily calculate the phase shift due to the boundary condition as

$$\tan\delta_{\pm}(k) = \frac{k}{E^{(\pm)}\cos\theta'_1 - m} \quad (A5)$$

This is equal to $\pm \tan\theta'_1$ for $k \to \infty$. If we adopt the convention that $\delta_{\pm}(k \to \infty) = \pm \theta'_1$ we can easily follow the evolution of $\delta_{\pm}(0)$ as θ'_1 increases from zero. For $\theta'_1 < \pi/4$, $\delta_+(0)$ is zero. At $\theta'_1 = \pi/4$ it discontinuously changes to $\pi/2$ [there is now a bound state exactly at the edge of the positive-energy continuum—the famous exception to the $\delta(0) = n\pi$ rule¹⁶]. For $\theta'_1 > \pi/4$ we find that $\delta_+(0) = \pi$ so it is keeping track of the state lost from the positive-energy continuum. $\delta_-(0)$ remains zero, until the lower continuum receives the ejected state at $\theta'_1 = 3\pi/4$, when it changes to $(-\pi)$ —all in accord with Eq. (2.24). We can use Eq. (2.16) to calculate the charge in the neighborhood of the boundary and confirm that the charge expelled to the left is indeed all caught there when we leave $\theta_1 = 0$.

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