explain our experimental result. A more detailed experiment and/or a new theory is necessary to the final determination of ABC.

The authors are greatly indebted to Dr. Inoue and Professor Nakayama of the Kyushu University for their valuable discussion and also for communicating their results to us prior to publication. This work was supported in part by the Kurata Research Grant.

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Continuum Quantum Field Theory for a Linearly Conjugated Diatomic Polymer with Fermion Fractionization

R. Jackiw and G. Semenoff

Center for Theoretical Physics, Laboratory for Nuclear Science and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

(Received 20 December 1982)

The recently proposed model Hamiltonian for a linearly conjugated diatomic polymer is studied in the continuum limit in which there emerges a field-theoretic Dirac Hamiltonian, exhibiting charge fractionization into irrational numbers, just as in the discrete model.

PACS numbers: 72.15.Nj, 11.10.Ef, 61.40.Km

There has appeared in this journal a Letter[1] describing a diatomic model polymer which supports solitons and the concomitant charge fractionization, with charge values that are irrational numbers, given by a transcendental function of the energy difference between energy levels of the two atomic constituents. This generalizes earlier work on polyacetylene, where the two atoms are identical (the energy difference vanishes) and the fractionization is $\frac{1}{2}$ per spin degree of freedom.[2] In a sense it also generalizes work on commensurate Peierls insulators, where the charge fraction is a rational number.[3]

Here we discuss the relation of this new investigation in condensed-matter physics[1] to parallel research in continuum quantum field theory. Fractionized fermion charge $\frac{1}{2}$ was found in a one-dimensional charge-conjugation–symmetric Hamiltonian, describing integer-charged and spinless fermions interacting with a soliton.[4] For a more general Hamiltonian without charge-conjugation symmetry, the fraction is an irrational number, parametrized by the magnitude of charge-conjugation–invariance violation.[5] The continuum charge-conjugation–symmetric Hamiltonian[4] arises as the continuum limit[6] of the discrete Su-Schrieffer-Heeger Hamiltonian,[2] which describes polyacetylene.[7] By taking the continuum limit of the Rice-Mele Hamiltonian relevant to a diatomic polymer,[1] we arrive at a Hamiltonian, violating charge-conjugation invariance, which is a particularly simple realization of the examples envisioned in Ref. 5, and can be thoroughly analyzed.[8] The analysis is especially beautiful, being very general, not relying on details of the Hamiltonian nor on the soliton profile, but rather using topological (asymptotic) properties.

Reference 1 posits the following model (RM) Hamiltonian,

$$H_{\rm RM}=H_{\rm phonon}+\alpha\sum_j a_j^\dagger a_j-\sum_j t_{j+1,j}(a_j^\dagger b_{j+1}+b_{j+1}^\dagger a_j)-\alpha\sum_l b_l^\dagger b_l-\sum_l t_{l+1,l}(b_l^\dagger a_{l+1}+a_{l+1}^\dagger b_l), \quad (1)$$

as a description of a diatomic linear chain of $N/2$ $(N\to\infty)$ atoms of type A (odd sites, labeled by j) and $N/2$ atoms of type B (even sites, labeled by l). Operators $a_j^\dagger, a_j$ and $b_l^\dagger, b_l$ are fermion creation and destruction operators at the A and B atomic sites. (We ignore spin, which is a passive label.) The hopping amplitude $t_{n+1,n}$ ($n=j$ or l), for the transfer of a fermion between neighboring sites, is taken to be linear in the phonon field y_n:

$$t_{n+1,n}=t_0-\gamma(y_{n+1}-y_n). \quad (2)$$

Energy levels of the two atomic constitutents are assumed to be uniformly displaced, one relative to the other, by $2\alpha=E_A-E_B$. $H_{\rm phonon}$, which governs phonon dynamics, will henceforth be ignored; i.e., we shall consider the fermions as moving in a prescribed, external phonon field.

To pass to the continuum, we define

$$a_j\equiv(-1)^{j/2}(2s)^{1/2}U(js),\quad b_l\equiv(-1)^{l/2}(2s)^{1/2}V(ls),\quad y_n\equiv(-1)^n\varphi(ns), \quad (3)$$

where s is the lattice spacing. Consequently one may rewrite (1) as

$$\begin{aligned}H_{\rm RM}=&-4it_0s^2\sum_n[U^\dagger(2ns+s)V'(2ns+s)+V^\dagger(2ns)U'(2ns)]\\&+2\alpha s\sum_n[U^\dagger(2ns+s)U(2ns+s)-V^\dagger(2ns)V(2ns)]\\&+4i\gamma s\sum_n\varphi(ns)[U^\dagger(ns)V(ns)-V^\dagger(ns)U(ns)]. \quad (4)\end{aligned}$$

Here we have further defined

$$\begin{aligned}&2sU'(2ns)\equiv U(2ns+s)-U(2ns-s),\quad 2sV'(2ns+s)\equiv V(2ns+2s)-V(2ns),\\&2U(2ns)\equiv U(2ns+s)+U(2ns-s),\quad 2V(2ns+s)\equiv V(2ns+2s)+V(2ns).\end{aligned} \quad (5)$$

It also follows that

$$\begin{aligned}\sum_n U^\dagger(2ns)U(2ns)&=\sum_n\tfrac14U^\dagger(2ns+s)[2U(2ns+s)+U(2ns+3s)+U(2ns-s)]\\&=\sum_n U^\dagger(2ns+s)U(2ns+s)+O(s). \quad (6a)\end{aligned}$$

Similarly one easily proves

$$\sum_n V^\dagger(2ns+s)V(2ns+s)=\sum_n V^\dagger(2ns)V(2ns)+O(s), \quad (6b)$$

$$\sum_n[U^\dagger(2ns)V'(2ns)+V^\dagger(2ns+s)U'(2ns+s)]=\sum_n[U^\dagger(2ns+s)V'(2ns+s)+V^\dagger(2ns)U'(2ns)]+O(s). \quad (6c)$$

This allows us to present (4), up to terms of order s, as

$$\begin{aligned}H_{\rm RM}=&-(2ist_0)s\sum_n[U^\dagger(ns)V'(ns)+V^\dagger(ns)U'(ns)]+\alpha s\sum_n[U^\dagger(ns)U(ns)-V^\dagger(ns)V(ns)]\\&+(4i\gamma)s\sum_n\varphi(ns)[U^\dagger(ns)V(ns)-V^\dagger(ns)U(ns)]. \quad (7)\end{aligned}$$

In the continuum limit $ns\to x$; $s\sum_n\to\int dx$; $U(ns)$, $U'(ns)$, $V(ns)$, $V'(ns)$, and $\varphi(ns)\to U(x)$, $dU(x)/dx$, $V(x)$, $dV(x)/dx$, and $\varphi(x)$, respectively. Thus we find

$$H_{\rm RM}\to\int dx\{2st_0\Psi^\dagger\sigma^1 i^{-1}d\Psi/dx-4\gamma\varphi\Psi^\dagger\sigma^2\Psi+\alpha\Psi^\dagger\sigma^3\Psi\},\quad \Psi(x)=\begin{pmatrix}U(x)\\V(x)\end{pmatrix}, \quad (8a)$$

where σ^i are Pauli matrices. By reabsorbing constants, and redefining the spinor $\Psi\to2^{-1/2}(1+i\sigma^3)\Psi$, we conclude that the continuum version of the RM Hamiltonian is proportional to

$$H=\int dx\{\Psi^\dagger\sigma^2i^{-1}d\Psi/dx+\Psi^\dagger\sigma^1\Psi\varphi+\epsilon\Psi^\dagger\sigma^3\Psi\}; \quad (8b)$$

or in first-quantized form, the Hamiltonian is a one-dimensional Dirac operator in the external field φ:

$$\hat H(\varphi)=\alpha p+\beta\varphi+\sigma^3\epsilon,\quad \alpha=\sigma^2,\quad \beta=\sigma^1,\quad p=i^{-1}d/dx. \quad (9)$$

Charged-conjugation symmetry would be present if there existed a unitary matrix which anticommutes with $\hat{H}(\varphi)$. But no such matrix can be constructed; we may say that ϵ, which is a measure of the energy difference in the level structure of the two atoms, is the charge-conjugation–symmetry breaking parameter: in its absence, σ^3 anticommutes with $\hat{H}(\varphi)$. Thus (9) is of the general form considered in Ref. 5, and in particular the special case of constant, rather than position-dependent, symmetry-breaking parameter was analyzed in Ref. 8.

In order to compute the charge, we need the eigenmodes of (9) in the presence of a soliton, $\varphi(x)=\varphi_s(x)$, and in its absence, i.e., in the "vacuum," $\varphi=\varphi_0=\text{const}$, $|\varphi_0|=\mu$:

$$\hat{H}(\varphi_0)\psi_E{}^0=E^0\psi_E{}^0,\quad \hat{H}(\varphi_s)\psi_E{}^s=E^s\psi_E{}^s. \tag{10}$$

The charge density at level E is $\rho_E(x)=\psi_E{}^\dagger(x)\times\psi_E(x)$, and the physical charge density is got by integrating ρ_E over all negative E, since the negative energy levels are filled:

$$\rho(x)=\int_{-\infty}^0 dE\,\rho_E(x). \tag{11}$$

Finally the soliton charge is obtained by integrating the charge density in the soliton field over all x, but to avoid an infinity, we must subtract a similar integral of the charge density when no soliton is present:

$$Q=\int dx\,\{\rho^s(x)-\rho^0(x)\}. \tag{12}$$

It is possible to evaluate (12) completely, without specifying the soliton profile φ_s. All we need to know about φ_s is that it interpolates between opposite "vacuum" values as x passes from $-\infty$ to $+\infty$:

$$\varphi_s(x)\xrightarrow[x\to\pm\infty]{}\pm|\varphi_0|=\pm\mu. \tag{13}$$

We now study the energy eigenmodes (10). The vacuum problem is trivial: The wave functions are plane waves and the spectrum is continuous, beginning at $\pm(\mu^2+\epsilon^2)^{1/2}$; $E^0=\pm(k^2+\mu^2+\epsilon^2)^{1/2}$.

When the soliton is present, let us note first the existence of a discrete bound state at $E^s=\epsilon$ (without loss of generality we take $\epsilon>0$). The wave function is proportional to

$$\begin{pmatrix}\exp[-\int^x dx'\,\varphi_s(x')]\\ 0\end{pmatrix}.$$

This is normalizable, precisely because φ_s tends to opposite limits at opposite ends of the real line.[9] To proceed we write ψ_E as $\binom{u}{v}$ and find that u satisfies a Schrödinger-like equation, while v is determined by u:

$$\begin{aligned}&(-\partial_x{}^2+\varphi^2-\varphi')u=(E^2-\epsilon^2)u,\\ &v=(E+\epsilon)^{-1}(\partial_x+\varphi)u.\end{aligned} \tag{14}$$

The "potential" is $\varphi^2-\varphi'$, which tends to μ^2 as $x\to\pm\infty$ in the presence of the soliton, and is identical to μ^2 in its absence.

With a soliton field, Eq. (14) possesses a bound state, $u^s(x)=\exp[-\int^x dx'\,\varphi_s(x')]$; this is just the Dirac bound state, previously identified. We shall assume that the soliton profile is sufficiently weak so that (14) supports no other bound states. (The subsequent development is easily modified if other bound states are present.) The remaining eigenmodes of (14) lie in the continuum, which begins at $\pm(\mu^2+\epsilon^2)^{1/2}$, $E^s=\pm(k^2+\mu^2+\epsilon^2)^{1/2}$.

It is now straightforward to construct the negative-energy solutions to the Dirac equations (10). Thus in the presence or absence of the soliton we have

$$\begin{aligned}&\psi_k=\begin{pmatrix}[(E+\epsilon)/2E]^{1/2}u_k\\ -[2E(E+\epsilon)]^{-1/2}(\partial_x+\varphi)u_k\end{pmatrix},\\ &\hat{H}(\varphi)\psi_k=E\psi_k,\quad E=-(k^2+\mu^2+\epsilon^2)^{1/2},\end{aligned} \tag{15}$$

where u_k is the properly normalized continuum solution to the Schrödinger equation. The charge density at (negative) E is given by

$$\begin{aligned}\rho_k(x)&=[(E+\epsilon)/2E]|u_k(x)|^2+[2E(E+\epsilon)]^{-1}|(\partial_x+\varphi)u_k(x)|^2\\ &=|u_k(x)|^2+[4E(E+\epsilon)]^{-1}\partial x^2|u_k(x)|^2+[2E(E+\epsilon)]^{-1}\partial_x[|u_k(x)|^2\varphi(x)]\end{aligned} \tag{16}$$

with the second equality following from the first, as a consequence of (14). The soliton charge is the integral over all x and k of the above evaluated with $\varphi=\varphi_s$, minus a similar integral in the vacuum; but in the vacuum, $|u_k|^2$ is constant, as is φ, and so the last two terms in (16) vanish. Thus

$$\begin{aligned}Q=&\int dx\int_{-\infty}^{\infty}\frac{dk}{(2\pi)}[|u_k{}^s(x)|^2-|u_k{}^0(x)|^2]\\ &+\int_{-\infty}^{\infty}\frac{dk}{(2\pi)}\frac{1}{4E(E+\epsilon)}[\partial_x|u_k{}^s(x)|^2+2|u_k{}^s(x)|^2\varphi_s(x)]\Big|_{x=-\infty}^{x=\infty}.\end{aligned} \tag{17}$$

The double integral can be evaluated by completeness: The $u_k^{\,0}$ represent *all* the Schrödinger modes in the vacuum, while the $u_k^{\,s}$ are *one short* of being complete in the soliton sector, since the normalized bound state is not among them. Hence the first term contributes -1 to Q. To evaluate the second term in (17), one needs the Schrödinger eigenmodes in the presence of a soliton, but only at $x=\pm\infty$. These may be given in terms of transmission and reflection coefficients:

$$\begin{aligned} u_k^{\,s}(x) &\xrightarrow[x\to\infty]{} Te^{ikx}, \\ u_k^{\,s}(x) &\xrightarrow[x\to-\infty]{} e^{ikx}+Re^{-ikx}. \end{aligned} \tag{18}$$

Thus, upon dropping oscillatory terms, we are left with

$$Q=-1+\int_{-\infty}^{\infty}\frac{dk}{2\pi}\,\frac{\mu}{2E(E+\epsilon)}[|T|^2+(|R|^2+1)], \tag{19a}$$

where the plus sign between the contributions at $x=\infty$ and at $x=-\infty$ arises because of sign reversal in $\varphi_s(x)$. Unitarity, $|T|^2+|R|^2=1$, permits a final evaluation

$$Q=-\pi^{-1}\tan^{-1}(\mu/\epsilon). \tag{19b}$$

This is a special case of the formula derived in Ref. 5, by an approximate method for a more general Hamiltonian, and is equivalent to the results of Ref. 1. Note that in the limit $\epsilon\to 0$, the charge-conjugation–symmetric value is regained[2,4]: $Q|_{\epsilon=0}=-\frac{1}{2}$.

One may even determine the charge density, when an explicit soliton profile is chosen. For example for $\varphi_s(x)=\mu\tanh\mu x$, we have

$$u_k(x)=-(1+ik/\mu)^{-1}e^{ikx}(\tanh\mu x-ik/\mu), \tag{20a}$$

$$\begin{aligned}\tilde\rho(x)&\equiv\int_{-\infty}^{\infty}\frac{dk}{(2\pi)}[\rho_k^{\,s}(x)-\rho_k^{\,0}(x)]\\ &=\left[-\frac{1}{2\pi}\tan^{-1}\frac{\mu}{\epsilon}\right]\partial_x\tanh\mu x=\frac{Q}{2\mu}\,\partial_x\varphi_s(x).\end{aligned} \tag{20b}$$

Finally we remark that the present results may also be derived by sophisticated mathematical procedures, based on index and spectral-flow theory of differential operators.[10] Thus the description of a diatomic polymer ranges from condensed-matter physics, to quantum field theory, and even to mathematics, providing a striking example of these disciplines' unity when they are used to describe natural phenomena.

We thank Dr. M. Rice for informing us of his results. This research is supported in part through funds provided by the U. S. Department of Energy under Contract No. DE-AC02-76ERO3069 and by the Natural Sciences and Engineering Research Council of Canada.

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