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FRACTIONALLY CHARGED EXCITATIONS IN QUASI-ONE-DIMENSIONAL SYSTEMS

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Recent theoretical studies have shown that in quasi-one-dimensional conductors having a Peierls distortion of commensurability index n (ratio of the distortion period to lattice spacing), there exist excitations whose charge is $Q = \bullet \frac{2e}{n}$ or $\bullet \frac{2e}{n} \pm e$. These excitations are kinks in the order parameter ψ describing the lattice distortion. In trans polyacetylene, n = 2 and Q = 0, ± e with spin $S = \frac{1}{2}$, 0 respectively. For n = 3 (e.g. TTF-TCNQ at 19Kb) $Q = \pm \frac{2}{3} e, \pm \frac{1}{3} e, \bullet \frac{4}{3} e$ with spin $S = 0, \frac{1}{2}, 0$ respectively. Electronic states localized at the kink have energies in the Peierls gaps. Properties of these stable fractionally charged objects are discussed.

I. INTRODUCTION

Fractionally charged excitations have often been considered in the past. Recently, however, it has been shown how a theory containing only fundamental particles of integer charged Q can lead to excitations having charge q which is a fraction of Q. In a continuum model of charge density waves in one-dimensional metals it was shown by Rice, Bishop, Krumhansl and Trullinger[1] that commensurability effects can stabilize kinks which carry a charge

$q = \Delta\theta/\pi$, where $\Delta\theta = 2\pi/n$, with n being the commensurability, e.g. n = 2 for a dimerized system, n = 3 for a trimerized system.

Independently, Jackiw and Rebbi[2] studied a relativistic field theory model in one dimension in which a spinless Dirac field is coupled to a self-interacting Bose field having two degenerate mean field ground states. They found that the model possessed soliton excitations which correspond to a change in the number of Dirac fermions in the vicinity of the kink being $\frac{1}{2}$. A c-number Fermion state at zero energy was found whose wavefunction was localized about the soliton. Depending on whether this state is occupied or not, the solitons would carry Fermion number $\pm \frac{1}{2}$, corresponding to charge $\pm e/2$.

Independently, J. Hubbard[3] studied a one-dimensional tight binding chain with very large on-site repulsions and weaker nearest neighbor interactions. In this limit, the problem splits into a set of spinless Fermions and a set of Heisenberg spins. Hubbard showed that for one electron per two sites on average (quarter filled band), an injected electron would split into two kinks, each of charge - e/2. A related problem will be discussed by M. J. Rice in the following paper.

Motivated by experiments on trans $(CH)_x$, Su, Schrieffer and Heeger (SSH)[4] studied a one-dimensional model of electrons hopping along a chain, with the hopping integral linearly modulated by lattice displacements. Similar studies were carried out by Rice.[5] Because of the Peierls distortion, the mean field ground state is degenerate. For the half-filled band (one electron per site on average) appropriate to undoped $(CH)_x$, the ground state is twofold degenerate. In this model, the symmetry breaking (loss of inversion symmetry in the phonon coordinates) is dynamically generated by the electron-phonon coupling as opposed to the imposed broken symmetry in the relativistic model of Jackiw and Rebbi. For the $(CH)_x$ model, it was found that there are low energy excited states corresponding to solitons which act as moving walls separating domains having different ground states, A and B. For each isolated soliton, an electronic state occurs in the center of the Peierls gap with

a wavefunction centered about the soliton, as in the Jackiw and Rebbi model.[2,6] An important difference, however, is that in $(CH)_x$ electrons of both spin orientation enter symmetrically in the Fermi sea so that the charge $q = \pm \frac{e}{2}$ is "spin masked," being doubled to $q = \pm e$. These states are of spin zero, while for $(CH)_x$ there is an added charge state of the soliton, $q = 0$ with spin $\frac{1}{2}$. Thus, instead of fractional charge being directly observable in $(CH)_x$, the effect appears as an interchange of the conventional charge-spin relations of electronic excitations in solids; instead of $q = \pm e$, $S = \frac{1}{2}$ for conventional electrons and holes, one has $q = \mp e$, $S = 0$ for charged solitons and $q = 0$, $S = \frac{1}{2}$ for neutral solitons. This breaking of the charge-spin relations of the underlying electron field is characteristic of the soliton excitations in a degenerate ground state system.

The one-third filled band (trimerized chain) was studied by Su and Schrieffer[7] using the SSH hamiltonian. A consequence of the threefold degeneracy of the ground state is the existence of two types of kinks, K_1 and K_2, each having three charge states: $\frac{2e}{3}$, $\frac{-e}{3}$, $\frac{-4e}{3}$ for K_1 and $\frac{-2e}{3}$, $\frac{e}{3}$, and $\frac{4e}{3}$ for K_2. The spin of the $\pm \frac{e}{3}$ kinks is $S = \frac{1}{2}$ while the other kinks have $S = 0$. Thus, spin no longer masks fractional charge for trimerized chains. Below I discuss the origin of these results derived in collaboration with W. P. Su.

II. TRIMERIZED CHAIN

We consider the model Hamiltonian

$$H = -\sum_{ns}\left[t_o - \alpha\left(u_{n+1} - u_n\right)\right]\left(c^{+}_{n+1,s}c_{n,s} + \text{H.c.}\right) + \frac{K}{2}\sum_{n}\left(u_{n+1} - u_n\right)^2 + \frac{M}{2}\sum_{n}\dot{u}_n^2 \qquad (1)$$

where u_n is the displacement of the n^{th} unit from its equilibrium position, c^{+}_{ns} is the π electron creation operator on the n^{th} unit and M is the

mass of one unit of the chain. K is an effective spring constant describing a harmonic approximation to the σ bond energy.

For the perfectly trimerized chain, we write in the (adiabatic) mean field approximation the most general function having the translation symmetry $\Delta n = 3$,

$$u_n = u \cos\left(\frac{2\pi}{3} n - \theta\right) \quad . \tag{2}$$

In Figure 1 the energy per site is plotted as a function of θ for three values of the amplitude $u = 0,\ 0.04\text{Å}$ and 0.07Å where, as an example, we have chosen the $(CH)_x$ parameters $t_o = 2.5$ eV, $\alpha = 4.81$ eV/Å, $K = 17.4$ eV/Å^2. The energy is minimized by $\theta - \frac{\pi}{6} = 0, \pm\frac{2\pi}{3}, \pm\frac{4\pi}{3}$, mod $\pm 2\pi, \ldots$ and $u_o \simeq 0.07\text{Å}$. As one can see, the minimum energy path to go between these minima is by changing the phase angle θ with the amplitude essentially fixed. This leads to a small barrier height of order Δ^3/t_o^2 and a soliton width $\xi_3 \sim \left(\frac{2t_o}{\Delta}\right)^2 a$. For the dimerized system, only the amplitude variable exists, and the

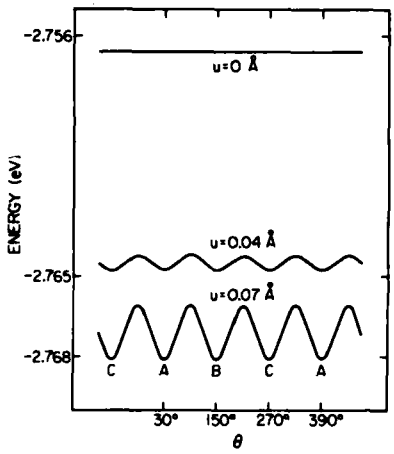

FIGURE 1 Total energy per site plotted as a function of the phase angle θ for three different values of the amplitude of trimerization u.

condensation energy passes through zero at the center of the kink, giving a barrier height of order Δ^2/t_o per site, and a soliton width $\xi_2 \sim \left(\frac{2t_o}{\Delta}\right) a$. Hence, the width of the trimerized soliton is larger than that of the dimerized system by the factor $\frac{2t_o}{\Delta} >> 1$.

To determine the charge and spin of the kinks in the one-third filled band case, one cannot use the charge conjugation symmetry derivation which has been used for the dimerized system since this symmetry gives no significant information in this case. Rather, one can use 1) a Green function method to determine the charge and spin density of the soliton or, 2) a simple but general argument based on translational invariance and charge conservation. It is this latter argument we present below.

Consider an infinitely long chain, $-\infty < n < \infty$, with $\theta_n - \frac{\pi}{6} = 0$, i.e. the A ground state. Suppose that θ_n is adiabatically deformed so that the chain remains in the A state for $-\infty < n < n_1$, is in the B phase $\left(\theta - \frac{\pi}{6} = \frac{2\pi}{3}\right)$ between n_1 and n_2, is in the C phase $\left(\theta - \frac{\pi}{6} = \frac{4\pi}{3}\right)$ between n_2 and n_3 and finally returns to the A state, phase shifted by a total of $2\pi\left(\theta - \frac{\pi}{6} = 2\pi\right)$. The change of θ_n near n_1, n_2 and n_3 need not be abrupt, but the transition region (soliton width) is assumed to be small compared to the spacings $n_2 - n_1$, and $n_3 - n_2$. There will be a certain width ξ_3 which will minimize the energy. As a result of this phase deformation, one has created 3 type I kinks (i.e. A $\rightarrow$ B, B $\rightarrow$ C, C $\rightarrow$ A).

To determine the charge and spin of the kinks, suppose that one constructs two surfaces, one at n_ℓ far to the left of n_1 and another at n_r far to the right of n_3. From global conservation of charge, we know that the total charge passing through these surfaces when θ_n is slowly deformed is the negative of the sum of the charges of the three solitons, ΔQ,

$$\int_{-\infty}^{\infty}[j_r(t) - j_\ell(t)]dt = -\Delta Q \qquad (3)$$

where j_r and j_ℓ are the electric current densities at the two surfaces. Since $\theta_n - \frac{\pi}{6}$ remains zero near n_ℓ, no current flows at this surface, while the charge passing the right-hand surface is the electronic charge in one unit cell of size 3a of the trimerized chain, i.e. - 2e and

$$\Delta Q = 2e \quad . \qquad (4)$$

However, from the invariance of H under translations ℓ a, it follows that all properties of the three kinks must be the same. Thus, the fundamental charge of type I kinks K_o is

$$\Delta Q = 3Q_{K_o} = 2e \qquad (5)$$

or

$$Q_{K_o} = \frac{2e}{3} \qquad (6)$$

A similar argument holds if the phase angle θ is decreased as one moves to the right so that one passes from A to C to B to A moving from left to right, with $\theta - \frac{\pi}{6} = 0, -\frac{2\pi}{3}, -\frac{4\pi}{3}, -2\pi$. The electric current is now in the reverse direction, and the fundamental charge of these type II kinks $\bar{K}_o$ (antikinks) is

$$Q_{\bar{K}_o} = -\frac{2e}{3} \qquad (7)$$

Since spin up and spin down states are identically occupied during the adiabatic deformation, the spin of K_o and $\bar{K}_o$ is zero,

$$S_{K_o} = S_{\bar{K}_o} = 0 \quad . \qquad (8)$$

As in the dimerized case, localized states

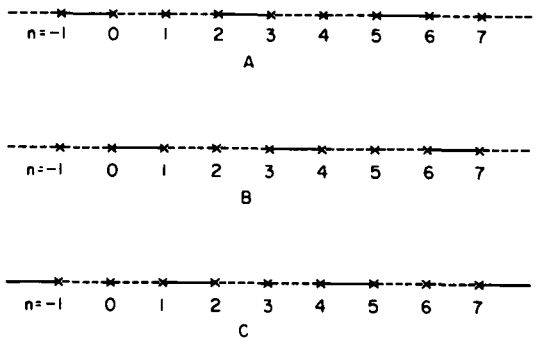

FIGURE 2 The three degenerate ground states of a perfectly trimerized chain.

are expected in the electronic energy gap connected with the solitons since states are missing from the valence band, leading to the fractional charge.

Using a Green function method one can determine the electronic spectrum in the presence of kinks. If one imposes a sharp kink K or antikink $\bar{K}$ on the system, one finds the spectrum shown in Figure 3. For the kink, there are two gap states ϕ_ℓ and ϕ_u located in the upper half of the lower gap and symmetrically in the lower half of the upper gap. Direct calculation of the fractional parentage coefficients of these states shows that for K, ϕ_ℓ

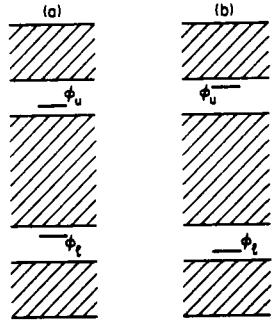

FIGURE 3 Gap states associated with (a) a sharp type-I kink and (b) a sharp type-II kink.

is derived 1/3 from the bottom band and 2/3 from the middle band, while ϕ_u comes 1/3 from the top band and 2/3 from the middle band. Since 1/3 of a state is removed from the bottom band by K and all valence band states remain filled as K is created, it follows that if ϕ_ℓ and ϕ_u are unoccupied (K_o), then the charge of K_o is $Q_{K_o} = 2/3\ e$, in agreement with (6) and (8). However, if ϕ_ℓ is singly occupied, then

$$Q_{K_1} = -\frac{e}{3} \quad , \quad S_{K_1} = \frac{1}{2} \tag{9}$$

and if ϕ_ℓ is doubly occupied, then

$$Q_{K_2} = -\frac{4e}{3} \qquad S_{K_2} = 0 \tag{10}$$

Similarly, the antikink $\bar{K}_o$ corresponds to having no holes in ϕ_ℓ, i.e. 2 electrons, so that its charge is

$$Q_{\bar{K}_o} = -2e + 2\left(\frac{2e}{3}\right) = -\frac{2}{3}\,e \quad , \tag{11}$$

in agreement with (7). In (11), the factor of two multiplying $\frac{2e}{3}$ arises from two spin orientations in accounting for the missing charge in the valence band due to the removal of 2/3 of a state per spin by an antikink from the lowest band. Since all states are spin paired for $\bar{K}_o$, it follows that

$$S_{\bar{K}_o} = 0 \tag{12}$$

Finally, if ϕ_ℓ is singly occupied in $\bar{K}_1$, then

$$Q_{\bar{K}_1} = +\frac{1}{3}\,e \quad , \quad S_{\bar{K}_1} = \frac{1}{2} \tag{13}$$

and if ϕ_ℓ is empty, then

$$Q_{\bar{K}_2} = +\frac{4}{3}\,e \quad , \quad S_{\bar{K}_2} = 0 \tag{14}$$

We see that K_ν and $\bar{K}_\nu$ act as antiparticles, having the same spin but reversed charge.

As in the dimerized case, there are constraints on creating solitons. If the chain is to be unaffected at infinity, topological constraints require that kinks must be created in pairs ($K\bar{K}$ or $\bar{K}K$), triplets (KKK or $\bar{K}\bar{K}\bar{K}$), or combination of these allowed sets. From the kink quantum numbers (Q,S),

	K_ν	$\bar{K}_\nu$
$\nu = 0$	$(2/3,0)$	$(-2/3,0)$
1	$(-1/3,\frac{1}{2})$	$(1/3,\frac{1}{2})$
2	$(-4/3,0)$	$(4/3,0)$

(15)

one can see that fractional charge and spin cannot be created globally but only locally. Hence, one would not be able to observe this type of fractional charge by measurements sampling the total charge of the system. Rather, the fractional charge reflects an internal distribution of an integer total charge of the system. One method for observing fractional charge in polymers is through the shot noise voltage fluctuation spectrum.

For n^{th} order commensurability, the primative kink quantum numbers are

$$Q_{K_o} = \frac{2e}{n} = -Q_{\bar{K}_o} \quad \text{and} \quad S_{K_o} = S_{\bar{K}_o} = 0 \ . \tag{16}$$

As above, K_o and $\bar{K}_o$ can be decorated by electrons and holes in the localized states.

III. REAL OR APPARENT FRACTIONAL CHARGE?

The question has been raised whether the fractional charge discussed above is a quantum mechanically sharp observable or simply the quantum average of two or more integer charges, the result of which is fractional.[8] In other words, if one can define a quantum operator Q_{op} which measures the charge of the soliton, then is the probability distribution $P(Q)$ of this operator in the one soliton sector

a delta function at the fractional kink charge Q_K

$$P(Q) = \delta(Q - Q_K) \tag{17}$$

or is it given by

$$P(Q) = \alpha_1 \delta(Q - Q_1) + \alpha_2 \delta(Q - Q_2) + \ldots . \tag{18}$$

where Q_1, Q_2, ... are integers, and only the expected charge is fractional

$$\langle Q_{op} \rangle = \sum_i \alpha_i Q_i = Q_K \quad ? \tag{19}$$

An example of apparent fractional charge, (18) and (19), is given by considering the H_2^+ ion. Suppose the electron is in the bonding (even parity) molecular orbital ψ_+ and the internuclear spacing is adiabatically increased to a very large value. In this limit ψ_+ reduces to a linear combination of 1s atomic orbitals φ centered on the two protons ℓ and r,

$$\psi_+ = \frac{1}{\sqrt{2}} \varphi_\ell + \frac{1}{\sqrt{2}} \varphi_r \quad . \tag{20}$$

If $Q_{op} = n_\ell$ is the occupation number for φ_ℓ, then

$$\langle \psi_+ | Q_{op} | \psi_+ \rangle = \frac{1}{2} \tag{21}$$

However, because Q_{op} has nonvanishing matrix elements between ψ_+ and the nearly degenerate antibonding state ψ_-

$$\psi_- = \frac{1}{\sqrt{2}} \psi_\ell - \frac{1}{\sqrt{2}} \varphi_r \tag{22}$$

it follows that ψ_+ is not an eigenfunction of Q_{op} and the mean square fluctuation is given by

$$\langle \psi_+ | Q_{op}^2 | \psi_+ \rangle - \langle \psi_+ | Q_{op} | \psi_+ \rangle^2 = | \langle \psi_+ | Q_{op} | \psi_- \rangle |^2 = \frac{1}{4} \tag{23}$$

For this simple example,

$$P(Q) = \frac{1}{2}\,\delta(Q) + \frac{1}{2}\,\delta(Q-1) \quad . \tag{24}$$

The usual quantum theory of measurement interpretation of this ficticious fractional charge is that while the average (expected) charge is fractional, only integer charge will be measured in any single experiment.

How is this related to the kinks? The essential point is that the off diagonal elements of the kink charge operator vanish exponentially in the limit of widely spaced kinks, rather than approaching a constant ($\frac{1}{2}$, see Eq. (23)) for the H_2^+ example. Therefore the one soliton state approaches an eigenfunction of Q_K for widely spaced kinks. This crucial difference arises from the fact there is a unique electronic ground state of $K\bar{K}$ for any spacing, with no low lying excited states, all excited states having an energy of order or greater than Δ. Furthermore, even these states are not excited by a very long wavelength potential since a slowly varying potential only couples to the total charge of the system in the vicinity of the kink. Therefore, the fundamental fractional charge of the kink is sharp and arises totally from the depletion of states from the filled valence band when a soliton is formed.

If Q_{op} measures the up spin charge on the soliton, then for K_o,

$$P(Q) = \delta(Q - \tfrac{1}{2}) \tag{24}$$

A totally separate but somewhat confusing question is the spacial distribution of charge located in the gap states. The discussion in the previous paragraph concerns configurations in which there are no electrons in the gap center states or when these states are completely filled. In this case there is no degeneracy, and a slowly varying field cannot admix excited states. Suppose, however, that we consider $K_1\bar{K}_o$ so that there is one spin up electron in the gap center state of K. This configuration is degenerate with K_oK_1; however, for finite spacing there is mixing which produces the analog of the ψ_+ state of H_2^+

$$\frac{1}{\sqrt{2}} K_1 \bar{K}_o + \frac{1}{\sqrt{2}} K_o \bar{K}_1 \quad . \tag{25}$$

In this case, the gap center electron fluctuates between K and $\bar{K}$ leading to a fluctuating K charge whose probability distribution is

$$P_K(Q) = \frac{1}{2} \delta(Q - \tfrac{1}{2}) + \frac{1}{2} \delta(Q + \tfrac{1}{2}) \quad , \tag{26}$$

which is to be compared with (24) showing a sharp distribution at $Q = \frac{1}{2}$. Clearly, the fractional charge associated with the vacuum deficit (or vacuum polarization) is a sharp quantum number, and it is this we refer to when discussing fractional charge. A ficticious fractional charge can enter from a totally different and uninteresting effect, namely that analogous to charge fluctuations in H_2^+ .

IV. CONCLUSION

While the noninteger charge effects discussed above will be screened by the dielectric constant of the medium, as in any solid the net charge macroscopically carried is the unscreened charge. The shot noise experiment should measure this charge. Fractionalized quantum numbers may be observable in other systems, such as domain walls in magnets and ^{3}He textures.[9] Recently, Goldstone and Wilczek[10] have shown how these ideas can be generalized to relativistic field theories in higher dimensions.

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