Fractional charge, a sharp quantum observable

S. Kivelson and J. R. Schrieffer
Institute for Theoretical Physics and Department of Physics, University of California, Santa Barbara, California 93106
(Received 28 December 1981)

The magnitude of quantum fluctuations of the charge of a fractionally charged soliton is calculated. The soliton charge operator is defined as $\hat{Q}_s = \hat{Q}_f - \langle 0 | \hat{Q}_f | 0 \rangle$, where $\hat{Q}_f$ is the integral of the charge-density operator sampled by a function f peaked at the position of the soliton, and falling smoothly to zero on a scale L. $|0\rangle$ is the ground state of the system in the absence of solitons. It is shown that the mean-square fluctuation of $\hat{Q}_s$ taken about its fractional average value Q_s vanishes as $O(\xi_0/L)$ for $L >> \xi_0$, where ξ_0 is the width of the soliton. Thus, as $L \to \infty$, the soliton is an eigenfunction of the charge operator with fractional eigenvalue. We also show that the portion of the charge fluctuations that are due to the soliton falls as $\exp(-L/\xi_0)$ as $L \to \infty$. Nonetheless, the charge of the entire system, including all solitons, is integral.

I. INTRODUCTION

Recently, Su and Schrieffer[1] (SS) deduced that in quasi-one-dimensional charge-density-wave (CDW) systems of commensurability $n=3$, there exist soliton excitations of charge $Q_s = \pm e/3$, $\pm 2e/3$, and $\pm 4e/3$ and spin $\frac{1}{2}$, 0, and 0, respectively. These tively. These results are consistent with the fermion number $\frac{1}{2}$ solitons discovered by Jackiw and Rebbi[2] for a one-dimensional Dirac field coupled to a φ^4 bose field and with solitons having peculiar charge-spin relations discovered by Su, Heeger, and one of the present authors[3-5] for the linear polymer $(CH)_x$, an $n=2$ CDW system. For general commensurability n, the simple counting arguments of SS associate with a soliton a fractional charge eN/n where N is the number of allowed spin polarizations. While the expectation value of the soliton charge was confirmed to be fractional using charge conjugation arguments[1] and by direct calculation for the $n=2$ and $n=3$ cases, questions have been raised[6] as to whether the charge of a soliton is in fact a sharp quantum observable. That is, are the quantum fluctuations of the soliton charge about its fractional average value vanishingly small or is the fractional value Q_s simply a quantum average of several integer values? In the latter case, each individual measurement of the charge would yield an integer value, and only the mean of these observed values would be fractional. More precisely, one may ask if an operator $\hat{Q}_s$ exists such that (1) the state $|s\rangle$ containing a soliton of fractional charge Q_s is an eigenfunction of $\hat{Q}_s$,

$$\hat{Q}_s | s \rangle = Q_s | s \rangle , \tag{1.1}$$

and (2) the force F on the soliton due to a slowly varying (screened) electric field, $\vec{E}$, is

$$F_s = Q_s \vec{E} . \tag{1.2}$$

A central complication in answering this question arises from the quantum fluctuations of the band electrons measured over any finite length of chain, whether or not the soliton is present. These fluctuations are precisely analogous to the vacuum fluctuations which complicate the definition of the charge on an electron. As in that case, the charge only has a well-defined value in the infinite-wavelength limit.

We are thus led to define the charge $\hat{Q}_f$ in a region sampled by a smoothly varying sampling function $f(x)$ of range L, for instance,

$$f(x) = e^{-x^2/L^2} , \tag{1.3}$$

so that

$$\hat{Q}_f = \int_{-\infty}^{\infty} \hat{\rho}(x) f(x)\, dx , \tag{1.4}$$

where $\hat{\rho}(x)$ is the charge-density operator. In order to show that the charge is a well-defined observable, it is necessary to show that: (1) the expectation value of the charge, $\langle s | \hat{Q}_s | s \rangle$, approaches a unique limit for large L for any $f(x)$ and (2) that the quantum fluctuations of the charge,

$$[\delta Q]^2 = \langle s | [\hat{Q}_s]^2 | s \rangle - [\langle s | \hat{Q}_s | s \rangle]^2 , \tag{1.5}$$

vanish for large L. The first property follows directly from results in Refs. 1–3 where it is shown that the charge associated with a soliton is localized in a region of width $2\xi_0$, so that for $L>>\xi_0$

$$\langle s\,|\,\hat{Q}_s\,|\,s\rangle = Q_s + O(e^{-L/\xi_0}) , \tag{1.6}$$

where ξ_0 is the correlation length defined in the next section. In Sec. II, two results concerning the nature of the quantum fluctuations are obtained. Firstly, it is shown that for any smoothly-varying sampling function of range L, such as the one in Eq. (1.3), the charge fluctuations vanish as

$$[\delta Q]^2 \propto (\xi_0/L) , \tag{1.7}$$

as long as $\xi_0 << L << d$, the soliton-antisoliton spacing. It is only in this limit that a sharp quantum number Q_s can be defined. It is, however, only in this limit that the macroscopically observable charge is defined. Secondly, it is shown that the charge fluctuations which are due to the presence of the soliton (as distinct from the vacuum fluctuations that are always present) fall off exponentially with L/ξ_0. Specifically, one finds

$$[\delta Q_s]^2 - [\delta Q_0]^2 \sim e^{-L/\xi_0} , \tag{1.8}$$

where for a given sampling function, $[\delta Q_s]^2$ and $[\delta Q_0]^2$ are the mean-square charge fluctuation in the presence and absence of a soliton, respectively. Thus, we see that the fluctuations of the soliton charge vanish exceedingly rapidly in the limit of large L.

II. QUANTUM FLUCTUATIONS OF THE SOLITON CHARGE

In this section we consider a specific model which allows us to calculate explicit upper bounds on the fluctuations of the soliton charge about its expected value, Q_s. We thus consider the continuum model of Takayama, Lin-Liu, and Maki[7] (TLM) which represents a system with commensurability $n=2$. For simplicity we consider the case of spinless electrons ($N=1$) so $Q_s=\pm\frac{1}{2}e$. The electronic part of the Hamiltonian for the continuum model is

$$\hat{H}^{\mathrm{TLM}} = \int dx\, \psi^\dagger(x) \left[-i\hbar v_F \sigma_z \frac{\partial}{\partial x} + \Delta(x)\sigma_x \right] \psi(x) , \tag{2.1}$$

where ψ is a two-component spinor field corresponding to right-going and left-going waves near the Fermi momentum, $\pm k_F$. The perfectly dimerized state has $\Delta(x)=\Delta_0$ while in the presence of a soliton $\Delta(x)=\Delta_0\tanh(x/\xi_0)$ where $\xi_0=\hbar v_F/\Delta_0$. In the following calculation we will adopt units $\hbar v_F=1$. The model in (2.1) is unbounded below unless a cutoff is introduced into the fermion spectrum. However, the charge fluctuations remain finite in the limit that the cutoff goes to infinity, so we will neglect the cutoff and compute the charge fluctuations in this limit.[8]

In the same spinor representation the charge density operator is

$$\hat{\rho}(x) = \psi^\dagger(x)\psi(x) . \tag{2.2}$$

The charge operator, $\hat{Q}_f$, is then defined in terms of $\hat{\rho}$ as in Eq. (1.4). The mean-squared fluctuation of the charge about its expectation value may be computed in the ground state $|G\rangle$ according to

$$[\delta Q]^2 = \sum_{\alpha\neq G} |\langle G\,|\,\hat{Q}_f\,|\,\alpha\rangle|^2 , \tag{2.3}$$

where $|G\rangle$ is the electronic ground state for a given lattice configuration, $\Delta(x)$, and $\{|\alpha\rangle\}$ is a complete set of excited states. The advantage of using the continuum model arises from the fact that all the one-electron wave functions are known (see Refs. 7 and 9), both in the case of a perfectly dimerized chain and of a soliton-bearing chain. Thus, an explicit expression for $[\delta Q]^2$ can be written in each case. In the perfectly dimerized case, $\Delta(x)=\Delta_0$, Eq. (2.5) can be written in terms of a double sum over the occupied valence-band wave functions, $|kv\rangle$, and the unoccupied conduction-band wave functions $|k'c\rangle$,

$$[\delta Q_0]^2 = \sum_k \sum_{k'} |\langle kv\,|\,\hat{Q}_f\,|\,k'c\rangle|^2 , \tag{2.4}$$

where

$$\langle x\,|\,kv\rangle = \frac{e^{ikx}}{\sqrt{2\epsilon_k\Omega}} \begin{bmatrix} \sqrt{\epsilon_k - k} \\ -\sqrt{\epsilon_k + k} \end{bmatrix} , \tag{2.5}$$

$$\langle x\,|\,kc\rangle = \frac{e^{ikx}}{\sqrt{2\epsilon_k\Omega}} \begin{bmatrix} \sqrt{\epsilon_k + k} \\ \sqrt{\epsilon_k - k} \end{bmatrix} , \tag{2.6}$$

ϵ_k is the one-particle excitation energy,

$$\epsilon_k = (k^2 + \Delta_0^2)^{1/2} , \tag{2.7}$$

and Ω is the total length of the chain. For large Ω, the sums in Eq. (2.4) can be converted into integrals,

$$[\delta Q_0]^2 = \int \frac{dk}{2\pi}\frac{dq}{2\pi}\,|F(2q)|\,\frac{[B(k,q)-\epsilon_k^2+q^2]}{B(k,q)}\,, \tag{2.8}$$

where $B(k,q)=\epsilon_{k+q}\epsilon_{k-q}$ and $F(k)$ is the Fourier transform of f,

$$F(k)=\int dx\, f(x)e^{ikx}\,. \tag{2.9}$$

In the presence of a soliton, $\Delta(x)=\Delta_0\tanh(\Delta_0 x)$, an analogous expression for the charge fluctuations, $[\delta Q_s]^2$, can be obtained from the known one-electron states. There are two contributions to δQ_s,

$$[\delta Q_s]^2=[\delta Q_b]^2+[\delta Q_g]^2\,. \tag{2.10}$$

$[\delta Q_b]^2$ involves only band-to-band excitations, with the midgap state associated with the soliton having the same occupation in the excited state, $|\alpha\rangle$, as in the ground state, $|G\rangle$, and $[\delta Q_g]^2$ only involves excitations to and/or from the midgap state. $[\delta Q_b]^2$ can be written as

$$[\delta Q_b]^2=\tfrac{1}{2}\int\frac{dk}{2\pi}\int\frac{dq}{2\pi}\left|\frac{[B(k,q)-\epsilon_k^2+q^2]}{B(k,q)}F(2q)-\frac{\Delta_0 T(2q)}{B(k,q)}\right|^2, \tag{2.11}$$

where

$$T(k)=\int dx\, e^{ikx}f'(x)\tanh(\Delta_0 x)\,, \tag{2.12}$$

$f'(x)$ is the derivative of f, while $[\delta Q_g]^2$ is given by

$$[\delta Q_g]^2=\int\frac{dk}{2\pi}\frac{\Delta_0}{4\epsilon_k^2}\,|S(k)|^2\,, \tag{2.13}$$

where

$$S(k)=\int dx\, e^{ikx}f'(x)\operatorname{sech}(\Delta_0 x)\,. \tag{2.14}$$

Note that we have not specified the occupancy of the midgap state. This is because for the case we are considering ($n=2$), the charge fluctuations are the same whether the state is occupied or not.

We will now use Eqs. (2.8)–(2.14) to establish the desired results. First we establish a rigorous upper bound to the charge fluctuations. To do this, we adopt a sampling function with a single characteristic length, L, so that $f(x)=g(x/L)$, where $g(0)=1$ and $g(x)\to 0$ as $x\to\pm\infty$. To establish an upper bound, we simplify the expression for δQ by using the inequalities

$$B(k,q)\le|\epsilon_k^2-q^2|+4\Delta^2q^2/B(k,q)\,,$$
$$B(k,q)\le\epsilon_k^2+q^2\,, \tag{2.15}$$

and

$$B(k,q)\ge\epsilon_k^2-q^2\,.$$

It is then straightforward to show that in the absence of a soliton,

$$[\delta Q_0]^2\le\left[\frac{\xi_0}{L}\right]A_0\,, \tag{2.16}$$

where A_0 is a number of order unity, given by the expression

$$A_0=\int\frac{dx}{8}[g'(x)]^2\,. \tag{2.17}$$

Similarly, in the presence of a soliton,

$$[\delta Q_s]^2\le\frac{\xi_0}{L}A_1+\left[\frac{\xi_0}{L}\right]^2A_2\,, \tag{2.18}$$

where

$$A_1=\int\frac{dx}{8}[g'(x)]^2[1+(7/2)\operatorname{sech}^2(\Delta_0 Lx)] \tag{2.19}$$

is equal to A_0 plus higher-order terms in ξ_0/L, and

$$A_2=\int\frac{dx}{4}\,|g''(x)g'(x)|^2\,. \tag{2.20}$$

Equations (2.16) and (2.18) show that the charge fluctuations vanish in the limit of large L. Note that this result depends critically on the existence of a gap, since ξ_0 diverges as the gap goes to zero. Indeed it is easy to show that for $\Delta_0=0$ (a one-dimensional metal) the charge fluctuations, $[\delta Q_m]^2$, approach a constant value in the limit of large L,

$$[\delta Q_m]^2\to\frac{f^2(0)}{2\pi}=\frac{1}{2\pi}\quad\text{as } L/\xi_0\to\infty\,. \tag{2.21}$$

The second result involves distinguishing the part of the charge fluctuations that are explicitly due to the presence of the soliton from the fluctuations that are present, even in the absence of a soliton. Thus, as in Eq. (1.8), we are led to define

$$[\Delta Q_s]^2=[\delta Q_s]^2-[\delta Q_0]^2\,. \tag{2.22}$$

To simplify the computation of $[\Delta Q_s]^2$ it is convenient to consider a sampling function, $f(x)$, such that $f(x)\approx 1$ over a region of width L and then falls to zero in a distance l. Specifically, we will consider a function $f(x)$ whose derivative is of the form

$$f'(x)=h(x+L/2)-h(x-L/2)\,, \tag{2.23}$$

where $h(x)$ is smooth and nonzero in a region of width l about the origin and $\int dx\, h(x)=1$. We would like to show that, for large $L >> \xi_0$, l, ΔQ_s falls exponentially to zero with increasing L. There are two sorts of terms that appear in the integrand of the integral expression for ΔQ_s

$$[\Delta Q_s]^2=\int \frac{dq}{2\pi}[I_1(q)+I_2(q)] \ . \qquad (2.24)$$

I_1 contains terms that are exponentially small for all q since it contains terms proportional to $|S(2q)|^2$ defined in Eq. (2.13) and $|\widetilde{T}(2q)|^2$,

$$\widetilde{T}(k)=\int dx\, e^{ikx}f'(x)[\tanh(\Delta_0 x)-\eta(x)] \ , \qquad (2.25)$$

where $\eta(x)=1$ for $x\geq 0$ and -1 for $x<0$. Because $f'(x)$ is localized in the vicinity of $x=\pm L/2$, T' is proportional to e^{-L/ξ_0} and S is proportional to $e^{-L/2\xi_0}$. Thus, the dominant contribution to I_1 comes from the term proportional to $|S(2q)|^2$. $I_2(q)$ contains terms that are not particularly small, but are rapidly oscillating functions of q,

$$I_2(q)=\frac{\Delta_0 H^2(2q)}{2}\left[\frac{\cos(4qL)}{\Delta_0^2+q^2} - \Gamma(q)\sin(4qL)\right] , \qquad (2.26)$$

where

$$H(k)=\int dx\, e^{ikx}h(x) \ , \qquad (2.27)$$

and

$$\Gamma(q)=\int \frac{dk}{\pi}q\frac{[B(k,q)-\epsilon_k^2+q^2]}{B^2(k,q)} \ . \qquad (2.28)$$

Because of the rapid variation of $I_2(q)$, the integral of I_2 is negligibly small. For instance, consider the case in which

$$h(x)=e^{-x^2/l^2}/\sqrt{\pi}l \ . \qquad (2.29)$$

It is easy to see that

$$\int dq\, I_2(q)\sim e^{-2L^2/l^2} \ , \qquad (2.30)$$

which is much smaller than the terms from I_1. We conclude that the dominant term in $[\Delta Q_0]^2$ is the term proportional to $|S|^2$; that is to say

$$[\delta Q_s]^2-[\delta Q_0]^2=[\delta Q_g]^2+O(e^{-2L/\xi_0}) +O(e^{-2L^2/l^2}) \ , \qquad (2.31)$$

where $[\delta Q_g]^2$ is the charge fluctuations due to the localized gap state defined in Eq. (2.13). For $h(x)$ given by Eq. (2.29), we can find $[\delta Q_g]^2$ explicitly:

$$[\delta Q_g]^2=e^{-L/\xi_0}\left[\frac{e^{-l^2/2\xi_0^2}}{2\sqrt{2\pi}}\left[\frac{\xi_0}{l}\right]\right] \times\left[1+O\left[\frac{\xi_0^2}{l^2}\right]\right] . \qquad (2.32)$$

III. CONCLUSION

The definition of the charge of a soliton requires care, since as in quantum field theory, two complications arise. First, the ground state of the system in the absence of solitons exhibits quantum vacuum fluctuations of the local charge which must be subtracted when considering the fluctuations due to the presence of a soliton. Secondly, the charge-form factor of a soliton is spacially extended over the width ξ_0 of the soliton. As is conventional in quantum field theory, it is useful to define the soliton charge operator $\hat{Q}_s$ as

$$\hat{Q}_s=\hat{Q}_f-\langle 0|\hat{Q}_f|0\rangle \ , \qquad (3.1)$$

where $|0\rangle$ is the ground state without solitons and

$$\hat{Q}_f=\int f(x)\hat{\rho}(x)dx \ , \qquad (3.2)$$

where $\hat{\rho}(x)$ is the linear charge density operator and $f(x)$ is a smoothly varying sampling function centered on the soliton and falling off on a scale L. $\hat{Q}_s$ is defined as the limit that L approaches infinity, with $L<<d$, the distance between solitons. Thus, $\hat{Q}_s$ samples the change in charge when a soliton is created in a given region of the system, with vanishing contribution from other solitons which may be created in other regions.

We have shown that not only is the expectation value of $\hat{Q}_s$ fractional in the presence of a soliton, but also that the change in the mean-square fluctuation of $\hat{Q}_s$ about its fractional mean vanishes as e^{-L/ξ_0} as $L\rightarrow\infty$. Furthermore, the mean-square vacuum fluctuations of $\hat{Q}_f$ in the absence of the soliton vanish as ξ_0/L as $L\rightarrow\infty$. It follows that, even if one does not remove the vacuum fluctuation contribution, the mean-square fluctuations of $\hat{Q}_s$ about its mean vanishes as $1/k_F L$ as $L\rightarrow\infty$. The soliton approaches an eigenstate of the charge operator $\hat{Q}_s$ as $L\rightarrow\infty$ as long as L is small compared to the spacing between solitons.

The remaining question is whether the operator $\hat{Q}_s$ couples to accessible external fields. Since the coupling of the chain to a (screened) electric field $E(x)$ is

$$\hat{H}' = -\int E(x)\hat{\rho}(x)\,dx \tag{3.3}$$

then if $E(x)$, like $f(x)$, is slowly varying in space it will couple to $\hat{Q}_s$, which is insensitive to the explicit form of $f(x)$ as long as $L >> \xi_0$. Thus, $\hat{Q}_s$ is the operator which enters in determining the electric force of F_s on a soliton due to a slowly varying (screened) electric field E,

$$\hat{F}_s(x) = \hat{Q}_s E(x)\ . \tag{3.4}$$

ACKNOWLEDGMENTS

We would like to thank Professor A. K. Kerman and Professor Weisskopf for raising the question of the quantum sharpness of fractional charge. Also, we would like to acknowledge many illuminating discussions with Dr. W. P. Su. This work was supported in part by National Science Foundation Grants Nos. DMR80-07432 and PHY77-27084.

---

[1]W. P. Su and J. R. Schrieffer, Phys. Rev. Lett. 46, 741 (1981).

[2]R. Jackiw and C. Rebbi, Phys. Rev. D 13, 3398 (1976).

[3]W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. 42, 1698 (1979); Phys. Rev. B 22, 2099 (1980).

[4]R. Jackiw and J. R. Schrieffer, Nucl. Phys. B 190, 253 (1981).

[5]M. J. Rice, Phys. Lett. 71A, 152 (1979).

[6]A. K. Kerman and V. Weisskopf (private communication).

[7]H. Takayama, Y. R. Lin-Liu, and K. Maki, Phys. Rev. B 21, 2388 (1980).

[8]S. Kivelson, T. K. Lee, Y. R. Lin-Liu, I. Peschel, and L. Yu, Phys. Rev. B 25, 4173 (1982).

[9]The charge fluctuations have also been computed in the discrete model of SSH (Ref. 3) where no artificial cutoff is required. All the continuum model results obtained in this paper can be obtained as the first terms in an asymptotic expansion for $[\delta Q]^2$ within the SSH model. [S. Kivelson (unpublished).]