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ON STATES, ON A LATTICE, WITH HALF INTEGRAL CHARGE

J.S. Bell

CERN -- Geneva

and

R. Rajaraman

Centre for Theoretical Studies, Indian Institute
of Science, Bangalore, India 560012

ABSTRACT

In certain molecular models, and related one dimensional field theories, localized objects appear with half integral expectation values of charge. We consider whether these states are eigenstates of charge ... with half integral eigenvalue. We find that it is indeed so for a suitably diffuse definition of the charge operator in question. This diffuse charge operator has a spectrum which approaches a continuum. The analysis is made on a lattice, to avoid divergence ambiguities, and on a finite length, which is only subsequently made large. The half integral charge phenomenon is not tied to solitons, but can arise also as an end effect.

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1. Introduction

In some very interesting papers [1-4] it has been shown that in certain models there appear states with half integral expectation value of charge in the neighbourhood of solitons. It has even been suggested that these states are eigenstates of charge ...with half integral eigenvalue. This has led to investigations of the charge fluctuations in the situations in question [5,6]. We have reported such an investigation in the context of the 1+1 dimensional continuum Dirac field theory [6]. Here we wish to make some further points in the context of a mathematical model related to the polyacetylene molecule [3,4]. This model is free from field theoretic infinities and ambiguities. We first show that with some change of notation it can be seen as a Kogut-Susskind-lattice [7] version of the Dirac theory (see also [8]). If we were then to impose periodic boundary conditions the discussion would follow closely our work on the continuum model. We now choose instead to work with a finite chain, whose ends are not identified. Boundary conditions are dictated by the Hamiltonian, and can not be imposed separately. It then appears that the phenomenon of half integral charge is not tied to solitons, but can appear also as an end effect. As before we find that the objects in question are eigenstates of partial charge operators only when these are defined with sufficient softness, or diffuseness, of the edges of the regions to which they refer.

2. Dirac equation from 'polyacetylene' model.

For our purposes the 'polyacetylene' model can be defined by the Hamiltonian

$$H = \sum_n \left(D^\dagger(n+1) D(n) + D^\dagger(n) D(n+1) \right) \left(u(n+1) - u(n) - \frac{1}{2a} \right) \quad (1)$$

where a is a parameter, $u(n)$ represents a given real c-number background field, and the D and $D^\dagger$ are fermion destruction and creation operators at lattice site n :

$$\{ D(n), D^\dagger(n') \}_+ = \delta_{n,n'} \quad (2)$$

As compared with Jackiw and Schrieffer we have omitted a trivial spin complication, and the dynamics of the phonon field u , and rescaled some variables.

Now let us retain n for even integers only, and use m for odd integers. Make the change of notation

$$C(n) \equiv i^n D(n) \quad B(m) \equiv i^{m+1} D(m) \\ \text{and let } u(m) \longrightarrow -u(m) \quad (3)$$

Then

$$H = \sum_n \left(B^\dagger(n+1) C(n) + C^\dagger(n) B(n+1) \right) \left(\frac{1}{2a} + u(n) + u(n+1) \right) \\ - \sum_m \left(C^\dagger(m+1) B(m) + B^\dagger(m) C(m+1) \right) \left(\frac{1}{2a} - u(m) - u(m+1) \right) \quad (4)$$

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Note the commutators

$$\begin{aligned} [B(m), H] &= \frac{-i}{2a} (C(m+1) - C(m-1)) + u(m) (C(m+1) + C(m-1)) + u(m-1) C(m-1) + u(m+1) C(m+1) \\ [C(n), H] &= \frac{i}{2a} (B(n+1) - B(n-1)) + u(n) (B(n+1) + B(n-1)) + u(n-1) B(n-1) + u(n+1) B(n+1) \end{aligned} \quad (5)$$

With some care of notation, these formulae hold even at the ends of the system. Suppose for definiteness that there are $2M+1$ lattice points, with M odd:

$$\begin{aligned} -M &\leq m < M \\ -M+1 &\leq n \leq M-1 \end{aligned} \quad (6)$$

Then the formulae hold at the end points as well if we set

$$C(M+1) = C(-M-1) = 0 \quad (7)$$

Note that these are not arbitrarily imposed boundary conditions, but simply a convenience in expressing the consequences of the Hamiltonian (4) in the form (5) when the summation in (4) is finite.

At this stage the model can be seen as a Kogut-Susskind lattice regulated version of 1+1 dimensional Dirac theory. Let $x = na$ or ma , and $L = 2Ma$, and consider the formal limit $a \rightarrow 0$ with L fixed. With the substitutions

$$C(n) \rightarrow C(x) \quad B(m) \rightarrow B(x)$$

$$4u(m), 4u(n) \rightarrow -\phi(x)$$

$$\sqrt{\frac{1}{2a}} \begin{pmatrix} B(x) \\ C(x) \end{pmatrix} \equiv \Psi(x) \quad (8)$$

the above commutators give the Dirac equation

$$[\Psi, H] = i \frac{\partial}{\partial t} \Psi = \left(-i \alpha \frac{\partial}{\partial x} - \beta \phi(x) \right) \Psi \quad (9)$$

with the representation of Dirac matrices

$$\alpha = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \beta = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (10)$$

and the boundary conditions, from (7),

$$C\left(\pm \frac{L}{2}\right) = 0 \quad (11)$$

Of course other boundary conditions could have been obtained By terminating the chain differently. For example identification of end points would have imposed periodicity.

Returning to the discrete lattice, the Hamiltonian (4) can be rewritten

$$H = \sum_{r=-M}^M \varepsilon_r A_r^\dagger A_r \quad (12)$$

in terms of new destruction and creation operators, A_r and $A_r^\dagger$,

related to the originals by

$$\begin{pmatrix} B(m) \\ C(n) \end{pmatrix} = \sum_{r=-M}^M A_r \begin{pmatrix} b^r(m) \\ c^r(n) \end{pmatrix} \quad (13)$$

where the (b^r, c^r) are a complete orthonormal set of wavefunctions

which solve equations derived from the commutators (5):

$$\begin{aligned} \mathcal{E}_r b^r(m) &= -\frac{1}{2a} (c^r(m+1) - c^r(m-1)) + u(m) (c^r(m+1) + c^r(m-1)) + u(m-1) c^r(m-1) \\ &\quad + u(m+1) c^r(m+1) \\ \mathcal{E}_r c^r(n) &= \frac{1}{2a} (b^r(n+1) - b^r(n-1)) + u(n) (b^r(n+1) + b^r(n-1)) + u(n-1) b^r(n-1) \\ &\quad + u(n+1) b^r(n+1) \end{aligned} \quad (14)$$

In the continuum limit these become the c-number Dirac equations derived from (9). Analogously with (11),

$$c^r(M+1) = c^r(-M-1) = 0 \quad (15)$$

The equations (14) have a 'charge-conjugation' symmetry such that for any solution

$$\begin{pmatrix} b^r(m) \\ c^r(n) \end{pmatrix}, \quad r = 1, 2, \dots, M \quad (16)$$

with eigenvalue ϵ_r there is another

$$\begin{pmatrix} b^{(-r)}(m) \\ c^{(-r)}(n) \end{pmatrix} = \sigma_3 \begin{pmatrix} b^r(m) \\ c^r(n) \end{pmatrix} \quad (17)$$

with eigenvalue $-\epsilon_r$, where

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Thus solutions with non-zero ϵ necessarily occur in pairs, and there are an even number of them. Since we must have an odd number, $2M+1$, altogether, there must then be a solution with zero energy for which c vanishes:

$$c^0(m) = 0 \quad \text{for all } m$$

Note that the zero energy solution exists whether or not the background field u is a topological soliton. There is one, and only one (because the difference equation is of first order) such zero energy solution. This simplicity depends on the particular way in which we terminated the system. It is not essential, but avoids some side issues.

The simplest case is that in which u does not vary with n or m :

$$u(n) = u(m) = -\mu/4 \quad \text{for all } n, m \quad (18)$$

where μ is a positive constant. Then the zero energy wavefunction is

$$\begin{pmatrix} b^0(m) \\ c^0(n) \end{pmatrix} = N_0 \begin{pmatrix} e^{Kma} \\ 0 \end{pmatrix} \quad (19)$$

where N_0 is a normalization constant, and κ is determined by

$$\tanh(\kappa a) = \mu a \quad (20)$$

This zero energy wavefunction is concentrated in a length of order $1/\mu$ at the $x = +L/2$ end of the system. The positive energy wavefunctions are

$$\begin{pmatrix} b^p(n) \\ c^p(n) \end{pmatrix} = N_p \begin{pmatrix} -\cos(pa(n+M+1) + \delta_p) \\ \sin(pa(n+M+1)) \end{pmatrix} \quad (21)$$

with

$$\cos \delta_p = \frac{\sin pa}{a \epsilon_p} \quad ; \quad \sin \delta_p = \frac{\mu}{\epsilon_p} \cos pa \quad (22)$$

and

$$\epsilon_p = \left[\frac{1}{a^2} \sin^2(pa) + \mu^2 \cos^2(pa) \right]^{1/2} \quad (23)$$

where p is determined by

$$pa(2M+2) = (1, 2, \dots, M) \pi \quad (24)$$

The normalization factor is, for $L \gg a$,

$$N_p = \left(\frac{2a}{L} \right)^{1/2} \quad (25)$$

The negative energy wavefunctions are determined by simply changing the sign of $c(n)$.

Closer to the soliton case of Jackiw et al is that in which u varies only in a neighbourhood

$$|x| < d/2$$

of the origin, where it changes sign. That is

$$\phi(x) = -\mu x/|x|, \quad |x| > d/2$$

If we specify also that

$$\phi(x) = -\phi(-x)$$

everywhere, then there is a reflection symmetry

$$\psi(x) \rightarrow \sigma_3 \psi(-x) \quad (26)$$

under which the wavefunction must have definite parity. Then the positive energy wavefunctions are again given by (21) for

$$x < -d/2$$

and by these same expressions with x replaced by $-x$, and change of sign of one component, for

$$x > +d/2$$

The wavenumbers p are determined by the requirement that these solutions, starting from either end, agree in the middle. The norms are again given by (25), assuming

$$L \gg d$$

The negative energy solutions are again obtained from those of

positive energy by changing the sign of $c(n)$. The new zero energy solution is of the form

$$\begin{pmatrix} b^0 \\ c^0 \end{pmatrix} = N_0' \begin{pmatrix} e^{-K|x|} \\ 0 \end{pmatrix} \quad (27)$$

for

$$|x| > d/2$$

3. Charge.

The charge operators per lattice site are

$$B^\dagger(m) B(m) \quad \text{and} \quad C^\dagger(n) C(n) \quad (28)$$

at odd and even sites respectively. This is only the electronic charge. In the original physical system there are also ionic charges, such that the physical system as a whole is more or less neutral. In omitting spin here we have only half as many electrons as originally, and neutrality is obtained by subtracting not one unit of charge, but one half, at each lattice site. In the field theory context this same subtraction is dictated by the decision to regard the charge of the Dirac sea of negative energy particles as unphysical, or by the wish to have the charge operator 'charge anticonjugate'. So we define subtracted charge operators

$$\rho(m) = B^\dagger(m) B(m) - 1/2, \quad \rho(n) = C^\dagger(n) C(n) - 1/2 \quad (29)$$

Consider now the particular state in which all the negative energy wavefunctions are occupied, while zero and positive energy states are unoccupied. Denote it by $|0\rangle$, i.e.

$$A_r |0\rangle = 0 \quad \text{for } r = 0, 1, \dots, M$$

$$A_r^\dagger |0\rangle = 0 \quad \text{for } r = -M, -M+1, \dots, -1.$$

The total subtracted charge of this state, Q , is

$$\begin{aligned} & (\text{number of occupied states}) - (\text{number of lattice sites})/2 \\ &= M - (2M+1)/2 \\ &= -1/2 \end{aligned}$$

It should be stressed that this half integrality is a trivial consequence of the definition (29) and our choice of an odd number of lattice sites. If we had chosen an even number of sites, or had identified the end points of the odd number (imposing periodicity, as we did previously in the continuum model [6]), the total charge would have been integral. The interesting thing is that the half integer can be considered to be localized where the zero energy wavefunction is localized.

To see this note that

$$\begin{aligned} \langle 0 | \rho(n) | 0 \rangle &= \left(\sum_{r < 0} |c^r(n)|^2 \right) - 1/2 \\ \langle 0 | \rho(m) | 0 \rangle &= \left(\sum_{r < 0} |b^r(m)|^2 \right) - 1/2 \end{aligned} \quad (30)$$

Now because of charge conjugacy (17)

$$\sum_{r < 0} |c^r(n)|^2 = \sum_{r > 0} |c^r(n)|^2 = \frac{1}{2} \left(\sum_{\text{all } r} |c^r(n)|^2 - |c^0(n)|^2 \right) \quad (31)$$

And because of completeness

$$\sum_{\text{all } r} |c^r(n)|^2 = 1 \quad (32)$$

So

$$\langle 0 | \rho(n) | 0 \rangle = -\frac{1}{2} |c^0(n)|^2 \quad (33)$$

and likewise

$$\langle 0 | \rho(m) | 0 \rangle = -\frac{1}{2} |b^0(m)|^2 \quad (34)$$

If we define a partial charge operator by

$$P = \sum \rho(n) + \sum \rho(m) \quad (35)$$

where the summation is over a subset of lattice sites, we have

$$\langle 0 | P | 0 \rangle = -\frac{1}{2} \left(\sum |c^0(n)|^2 + \sum |b^0(m)|^2 \right) \quad (36)$$

Provided only that the summation is over all sites where the zero energy wavefunction is appreciable, the normalization of that wavefunction implies

$$\langle 0 | P | 0 \rangle \approx -\frac{1}{2} \quad (37)$$

4. Charge fluctuations

Could the state $|0\rangle$ be an eigenstate of partial charge P , with

eigenvalue as well as expectation value half integral? When P is defined by summing over an even number of sites, the answer is immediately: no. For then, from (29), the eigenvalues are trivially integral.

More generally, consider the fluctuation

$$\langle 0 | \Delta^2 | 0 \rangle$$

where

$$\Delta \equiv P - \langle 0 | P | 0 \rangle \quad (38)$$

In terms of a complete set of excited states $|s\rangle \neq |0\rangle$,

$$\begin{aligned} \langle 0 | \Delta^2 | 0 \rangle &= \sum_s |\langle s | P | 0 \rangle|^2 \\ &= \sum_s |\langle s | \frac{dP}{dt} | 0 \rangle|^2 (E_s - E_0)^{-2} \end{aligned} \quad (39)$$

where

$$i \frac{dP}{dt} = [P, H]$$

The dP/dt form is convenient because for a given region dP/dt can be expressed in terms of currents across the boundaries. From (4)

$$[P(m), H] = \frac{1}{2a} (C^\dagger_{(m+1)} - C^\dagger_{(m-1)}) B(m) - (h.c.) + \dots$$

$$[P(n), H] = \frac{1}{2a} C^\dagger(n) (B(n+1) - B(n-1)) - (h.c.) + \dots \quad (40)$$

where... indicates terms which contain factors u , rather than $1/(2a)$,

which are relatively unimportant when

$$\mu a \ll 1$$

We will drop such terms hereafter. Carrying them along lengthens the expressions without changing the conclusions. Suppose, as is relevant in the case (19) with the zero energy wavefunction at one end of the system, that P is defined by summing ρ over lattice sites such that

$$\begin{aligned} m \geq \bar{m} \quad \text{and} \quad n \geq \bar{m} + 1 \\ \text{with} \quad M \gg M - \bar{m} \gg (\mu a)^{-1} \end{aligned} \quad (41)$$

Then

$$\begin{aligned} \langle 0 | \Delta^2 | 0 \rangle \\ = \sum_p \left(\frac{1}{2a} \right)^2 \left| \langle 0 | C^\dagger(\bar{m}-1) B(\bar{m}) - B^\dagger(\bar{m}) C(\bar{m}-1) | 0 \rangle \right|^2 (E_p - E_0)^{-2} \end{aligned} \quad (42)$$

The excited states s are formed by emptying one of the negative energy levels and occupying one of the positive energy levels (or the zero energy level, but we have supposed $\bar{m}$ out of range of this). Since the negative energy wavefunctions are obtained from those of positive energy just by changing the sign of one component, the result can be written as a sum of over pairs of positive energy levels:

$$\langle 0 | \Delta^2 | 0 \rangle = \sum_{p,q} \left(\frac{1}{L} \right)^2 \left| F(p,q,\bar{m}) \right|^2 (\epsilon_p + \epsilon_q)^{-2} \quad (43)$$

where (with the wavefunctions real)

$$\begin{aligned}
 F(p, q, \bar{m}) &\equiv \left(\frac{L}{2a}\right) \left(c^p(\bar{m}-1) b^q(\bar{m}) + b^p(\bar{m}) c^q(\bar{m}-1) \right) \\
 &= \sin(pa(\bar{m}+M)) \cos(qa(\bar{m}+M+1) + \delta_q) + (p \leftrightarrow q)
 \end{aligned}
 \tag{44}$$

For

$$1 \gg pa, qa \gg \mu a$$

this simplifies to

$$F(p, q, \bar{m}) \approx \sin((pa+qa)(\bar{m}+M)) \tag{45}$$

Thus the quantity (43) is not only non zero, but diverges as does the integral

$$2 \int \frac{dp}{2\pi} \int \frac{dq}{2\pi} (\epsilon_p + \epsilon_q)^{-2}, \text{ for } L \rightarrow \infty, a \rightarrow 0 \tag{46}$$

However such large fluctuations, in sharply bounded regions, are just normal in quantum field theory. As is well known, the fluctuations are less in regions with diffuse boundaries...that is, for charges defined by weight functions that fall progressively, rather than immediately, to zero at the boundaries. Some such diffuseness can be incorporated by averaging over a range of values of $\bar{m}$ in $F(p, q, \bar{m})$:

$$F(p, q, \bar{m}) \longrightarrow \bar{F}(p, q, \bar{m}, \bar{n})$$

where

$$\bar{F}(p, q, \bar{m}, \bar{n}) \equiv \frac{1}{\bar{n}+1} \sum_{\bar{m}-\bar{n}}^{\bar{m}+\bar{n}} F(p, q, m) \tag{47}$$

Now F can be written in the form

$$F(p, q, m) = X \sin(pam + qam + \xi) + Y \sin(pam - qam + \theta) \quad (48)$$

where X, Y, ξ , θ , are independent of m, and X and Y are of order unity.

Then

$$\begin{aligned} \bar{F}(p, q, \bar{m}, \bar{n}) \\ = f(p, q, \bar{n}) X \sin(p\bar{a}\bar{m} + q\bar{a}\bar{m} + \xi) + g(p, q, \bar{n}) Y \sin(p\bar{a}\bar{m} - q\bar{a}\bar{m} + \theta) \end{aligned} \quad (49)$$

where

$$f(p, q, \bar{n}) = \frac{\sin((pa + qa)(\bar{n} + 1))}{(\bar{n} + 1) \sin(pa + qa)} \quad (50)$$

$$g(p, q, \bar{n}) = \frac{\sin((pa - qa)(\bar{n} + 1))}{(\bar{n} + 1) \sin(pa - qa)}$$

Then

$$\langle 0 | \Delta^+ | 0 \rangle < K \left\{ \sum_{p, q} \frac{1}{4L^2} (|f|^2 + |g|^2) (\epsilon_p + \epsilon_q)^{-2} \right\} \quad (51)$$

where K is a constant of order unity. In the limit $L \rightarrow \infty$,

$$\langle 0 | \Delta^2 | 0 \rangle < K \int_0^{\pi/2a} \frac{dp}{2\pi} \int_0^{\pi/2a} \frac{dq}{2\pi} (|f|^2 + |g|^2) (\epsilon_p + \epsilon_q)^{-2} \quad (52)$$

In the region of integration we have crude but sufficient bounds

$$\epsilon_p > (\mu+p)/4 \quad ; \quad \epsilon_q > (q+\mu)/4 \quad (53)$$

Noting that $|f|$ and $|g|$ are both symmetric about both the lines

$$(p+q) = \frac{\pi}{2a} \quad \text{and} \quad p-q = 0$$

then

$$\begin{aligned} & \langle 0 | \Delta^2 | 0 \rangle \\ & < \frac{8K}{\pi^2} \int_0^{\pi/2a} d(p+q) \int_0^{p+q} d(p-q) \frac{|f|^2 + |g|^2}{(p+q+2\mu)^2} \end{aligned} \quad (54)$$

Now divide the $(p-q)$ integration into two parts,

$$p-q < w^{-1} \quad \text{and} \quad p-q > w^{-1} \quad (55)$$

where

$$w \equiv 2(\bar{n}+1)a \quad (56)$$

In the first part use

$$|f| < 1 \quad , \quad |g| < 1 \quad (57)$$

and in the second part use

$$|g| \leq \frac{\pi}{|p-q|w} \quad , \quad |f| \leq \frac{\pi}{(p+q)w} \leq \frac{\pi}{|p-q|w} \quad (58)$$

Then finally

$$\langle 0 | \Delta^2 | 0 \rangle < \frac{8K}{\pi^2} \int_0^\infty d(p+q) \left[\frac{2/w + \pi^2/w}{(2\mu + p+q)^2} \right] \quad (59)$$

This bound, which is independent of a , goes to zero with $1/w$. By reducing the weight function, defining the partial charge, to zero sufficiently slowly, the fluctuations are completely suppressed. Of course we keep $L \gg w$.

The discussion of the soliton case (27) goes along similar lines. The partial charge of interest is then that in a length l , containing both kink and zero energy wavefunction,

$$l \gg d \quad , \quad \kappa l \gg 1$$

We come again to expressions of the form (38)(44). The fluctuations are again large for small a (twice as big as before because the region in question has two ends) However again with the sequence of limits

$$L \rightarrow \infty$$

$$l \rightarrow \infty$$

$$w \rightarrow \infty$$

the fluctuations are completely suppressed.

5. Concluding remarks

Whether the total charge is integral or not is a trivial matter of how much is subtracted in defining it. What is more significant is that in the neighbourhood of each zero energy wavefunction a half integer of charge is localized. Moreover this half integer is not just an expectation value, but even an eigenvalue of a partial charge operator covering the relevant region with sufficiently diffuse boundaries. It should be noted that the eigenvalues of such operators, far from being integral or half integral, actually form almost continua, corresponding to the variety of weights involved in constructing them from the site charges (29).

The phenomenon of half integral charge is not necessarily associated with solitons. In the case that we studied in detail here, it occurred even in the soliton-free sector, as an end effect. For definiteness we considered here the case of $2M+1$ lattice sites with M odd. Other choices could of course be made and analysed similarly. If M were even instead, b rather than c would vanish at the end points (in the continuum limit) and the zero energy wavefunction, in the kink-free case, would move to the other end of the chain. If the total number of sites were even rather than odd, b would vanish at one end and c at the other (in the continuum limit), and there would be no exactly zero energy solutions. There might or might not be two nearly zero energy solutions, in the soliton-free sector, depending on which end is which and the sign of μ .

As regards the total charge Q , summing over all n and m in (29), note that it is either integral for all states, or half integral for all states, depending on whether the total number of lattice sites is even or odd. For a given system there is no question of having integral total charge for some states and half integral for others.

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