Dyon Analogs in Antiferromagnetic Chains

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A close analogy is pointed out between dyons (particles with electric and magnetic charge) in grand-unified theories and solitons in antiferromagnetic chains. For nonzero topological angle θ, dyon electric charges are noninteger: $q=(n+\theta/2\pi)e$. An analogous phenomenon occurs in antiferromagnets with alternating interactions.

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The well-known reversed charge-spin states in polyacetylene[1] are a condensed-matter realization of a phenomenon first discovered in particle physics[2]: The fermionic ground state in the presence of a soliton can have a fractional fermion number. There is another well-known fractional effect connected with solitons in particle physics: Dyons in the presence of a nonzero topological angle, θ, have fractional electric charges $e(n+\theta/2\pi)$, where n is an integer.[3] It is the purpose of this Letter to point out a possible condensed-matter realization of this effect.

In unified gauge theories, the magnetic monopole appears as a time-independent classical solution.[4] The dyon is a more general time-dependent solution[5] (in temporal gauge) with **E**, the non-Abelian electric field, periodic and **B**, and non-Abelian magnetic field, the same constant field as before. This time dependence corresponds to a periodic gauge rotation. It can be parametrized by a collective coordinate $\beta(t)$, where β is an angular variable. The Lagrangean for β, in the absence of a topological term, is simply that of a rigid rotator: $L=(I/2)\dot\beta^2$ (where I, the moment of inertia, is a constant). The angular momentum variable conjugate to β is the rescaled electric charge, $l=q/e=I\dot\beta$. Thus the Hamiltonian for the electric charge, q, is $H=(q/e)^2/2I$ and, with the imposition of periodic boundary conditions on β, q/e has integer quantum numbers. The quantum states can be obtained by semiclassical quantization of the periodic classical solutions with frequency $\dot\beta=\omega=q/eI$. The fact that dyon states come in degenerate pairs of opposite electric charge is a consequence of CP (charge and parity) symmetry which reverses electric, but not magnetic, charges. A topological term, $\int d^4x(\theta/4\pi)\mathbf{E}\cdot\mathbf{B}$, can be added to the action. Since, in Euclidean space, this is a topological invariant, taking only values in, where n is an integer, the physics is expected to be periodic in θ. Since the topological term is a total derivative it has no effect in perturbation theory; it *does* produce effects $O(e^{-8\pi/g^2})$ as a result of instantons. However, it has an effect $O(1)$ on the dyon, because the quantity $\mathbf{E}\cdot\mathbf{B}$ is nonzero for a dyon. Since the topological term is odd under CP symmetry but even under C, dyons need no longer come in degenerate pairs with the same magnetic charge but opposite electric charge. There is still a pairing of dyons with opposite electric *and* magnetic charges. To calculate explicitly the effect of the topological term on dyons we observe[3] that the Lagrangean for the collective coordinate β is shifted by a term linear in θ and $\dot\beta$: $L=(I/2)\dot\beta^2-(\theta/2\pi)\dot\beta$. The breaking of CP or equivalently T invariance is manifest as is the fact that the added term is a total derivative. The momentum conjugate to β is shifted to $l=I\omega-\theta/2\pi$. The Hamiltonian becomes $H=(1/2I)\times(l+\theta/2\pi)^2$. The observable electric charge is *not el* now but is the unshifted quantity $eI\omega$, since external currents do not couple to the topological term. Thus the dyon electric charge is now fractional, $q=e(n+\theta/2\pi)$, where n is an integer. Furthermore, rotational states with opposite angular momentum, $\pm n$, correspond to classical motions with frequencies $(\pm n+\theta/2\pi)/I$ which are *not* opposite and correspondingly have different energies.

We now turn to a possible condensed-matter analog of fractionally charged dyons. Thus, consider an antiferromagnetic chain with Ising anisotropy:

$$H=J\sum_i[\mathbf{S}_i\cdot\mathbf{S}_{i+1}+aS_i^zS_{i+1}^z-b(S_i^z)^2] \qquad (1)$$

$$(J>0),\quad \mathbf{S}_i^2=s(s+1)$$

(we will use units in which $\hbar=1$). This Hamiltonian has a U(1) symmetry (rotation about the z axis) and two important discrete symmetries: time reversal T, $\mathbf{S}\to-\mathbf{S}$, and translation by one site P, $\mathbf{S}_i\to\mathbf{S}_{i+1}$. For a range of parameters with sufficiently large positive a and b, P and T are expected to be spontaneously broken to PT. In the large-s (semiclassical) limit the ground states are well approximated by the Néel states $\mathbf{S}_i=\pm s(-1)^i\hat{\mathbf{z}}$. Whenever a discrete symmetry is spontaneously broken in such a one-dimensional system one expects solitons to exist which interpolate between the ground states. The semiclassical soliton solution[6,7] (which will be constructed explicitly below) exhibits a rotation of the spins on even sites from the north to the south pole with some fixed (and arbitrary) polar angle as we move along the chain. (The spins on odd sites rotate from south to north.) This solution plays a role in the present discussion which is analo-

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gous to that of the magnetic-monopole classical solution. As in that case, there is a more general time-dependent solution.[7] The spins comprising the soliton may precess about the z axis (with a sense of precession which does *not* alternate from site to site; see Fig. 1). Exactly as before, one may introduce a collective coordinate, β, to parametrize this precession. The allowed precession frequencies $\dot{\beta}=\omega$ are integers, n. The symmetry responsible for the pairing of "dyon" states with opposite frequency is now PT which takes soliton into soliton but reverses the sense of precession. Let us now generalize the model of Mikeska[6] and Haldane[7] and consider a modified Hamiltonian in which PT is explicitly broken to T. It is known that dimerization can occur in one-dimensional antiferromagnets as a result of the spin-Peierls effect.[8] This leads to a shift in the Hamiltonian $H\rightarrow H+\alpha\sum_i(-1)^i\mathbf{S}_i\cdot\mathbf{S}_{i+1}$. (More generally, the anisotropic terms could pick up alternating pieces also. These could be included in the present analysis; I omit them for simplicity. In cases where both the anisotropy and the alternation are small, the alternating anisotropy may be second order in small quantities.) This extra term breaks P symmetry but preserves T; thus we might expect it to destroy the symmetry between dyons of opposite precession frequency. To understand how this can happen, note that the effect of the precession is to shift S_i^z by an amount δS_i which has a uniform sign. Then, to linear order in δS, the alternating term produces a shift in the energy of

$$\delta E=\alpha\sum_i[\delta S_{2i}(S^z_{2i+1}-S_{2i-1})-\delta S_{2i+1}(S^z_{2i+2}-S^z_{2i})].$$

Since the quantities $(S^z_{2i+1}-S^z_{2i-1})$ and $-(S^z_{2i+2}-S^z_{2i})$ have the same sign ($\pm$ for soliton or antisoliton) each term in δE has the same sign and so there is no possibility of a cancellation. Thus, remarkably, there is a favored sense of precession for a soliton determined by the sign of α. Of course an antisoliton prefers to precess in the opposite sense; the symmetry between soliton and antisoliton of opposite precession frequency is preserved (it is a consequence of T). We now turn to a quantitative analysis of this effect in the large-s (semiclassical) limit.

At large s we expect quantum fluctuations around the Néel ground states to be suppressed. Therefore we define[7,9] slowly varying fields

$$\boldsymbol{\phi}_{2i+1/2}=(\mathbf{S}_{2i+1}-\mathbf{S}_{2i})/2s,\quad \mathbf{l}_{2i+1/2}=(\mathbf{S}_{2i+1}+\mathbf{S}_{2i})/2\Delta \tag{2}$$

(where Δ is the lattice spacing). In the large-s continuum limit (formally $\Delta\rightarrow 0$) these obey the commutation relations and constraints of the fields and rotation generators of the O(3) σ model:

$$\begin{aligned}&[l^i(x),\phi^j(y)]=i\epsilon^{ijk}\phi^k(x)\delta(x-y),\\ &[l^i(x),l^j(y)]=i\epsilon^{ijk}l^k(x)\delta(x-y),\\ &[\phi^i(x),\phi^j(y)]=0,\quad \boldsymbol{\phi}^2=1,\quad \mathbf{l}\cdot\boldsymbol{\phi}=0.\end{aligned} \tag{3}$$

Solving for the spin variables $\mathbf{S}_i$ in terms of $\boldsymbol{\phi}$ and $\mathbf{l}_i$, substituting into the Hamiltonian, and expanding in the number of derivatives of the slowly varying fields, we obtain the large-s continuum Hamiltonian density:

$$H=\tfrac{1}{2}c\left\{g\left[\mathbf{l}+\frac{\theta}{4\pi}\boldsymbol{\phi}'\right]^2+g^{-1}\boldsymbol{\phi}'^2-\frac{m^2}{g}(\phi^z)^2\right\}, \tag{4}$$

where the coupling constant g is given by $g^{-1}=(s/2)[1-\alpha^2]^{1/2}$, the speed of "light" is $c=2\Delta sJ(1-\alpha^2)^{1/2}$, the symmetry-breaking mass is given by $m^2=(a+b)/2\Delta^2$, and the topological angle is $\theta=2\pi s(1+\alpha)$. The theory is invariant under Lorentz transformations with speed of light c. Thus c represents the maximum velocity of any excitation. We will generally set it equal to 1 in what follows. The Lagrangean density arising from Eq. (4) by a canonical transformation is

$$L=(1/2g)[\partial^\mu\boldsymbol{\phi}\cdot\partial_\mu\boldsymbol{\phi}+m^2(\phi^z)^2]+(\theta/4\pi)\boldsymbol{\phi}\cdot(\partial^\mu\boldsymbol{\phi}\times\partial^\nu\hat{\boldsymbol{\phi}})\epsilon_{\mu\nu}. \tag{5}$$

In imaginary time the last term in L is multiplied by i since it contains one time derivative. Thus it is a purely imaginary term in the action. This term is $i\theta n_v$, where n_v is the winding number of the sphere on which the field $\boldsymbol{\phi}$ is defined onto the two-dimensional position space (which is also equivalent to a sphere if we impose a fixed boundary condition at infinity). Thus n_v is always an integer, the vortex number, and therefore the physics is periodic

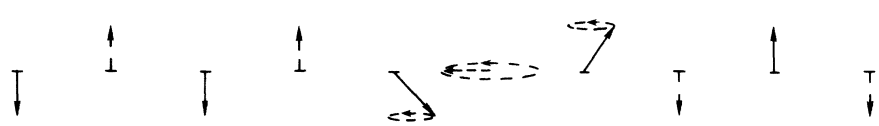

FIG. 1. A dyon occupying three sites. In the semiclassical limit, the dyon is spread over a very large number of sites.

in θ, the topological angle. Furthermore, this topological term is a total derivative and so has no effect in perturbation theory in $g(1/s)$. Thus the dependence on θ is exponentially small in $1/s$ and periodic. A physical interpretation of this periodic α dependence is given elsewhere.[10] The two classical ground states of the Hamiltonian of Eq. (4), $\phi^z = \pm 1$, correspond to the two Néel ground states of the spin chain. The T symmetry of the spin chain becomes the symmetry $\boldsymbol{\phi} \to -\boldsymbol{\phi}$, $t \to -t$ (time reversal) of the σ model and the P symmetry becomes $\boldsymbol{\phi} \to -\boldsymbol{\phi}$. ($P$ is not spatial parity but a type of internal parity or charge conjugation.) P is explicitly broken by the topological term except at $\theta = 0$ or π where $\exp(i\theta n_v)$ is invariant under $n_v \to -n_v$. T and P are spontaneously broken to TP in the Néel ground state (the latter only when it is a good symmetry, of course). The perturbative excitations predicted by this Hamiltonian can be read off by writing

$$\boldsymbol{\phi} = (\sqrt{g}\,\phi^x, \sqrt{g}\,\phi^y, [1 - g(\phi^x)^2 - g(\phi^y)^2]^{1/2})$$

and expanding in ϕ^x and ϕ^y. This gives the Lagrangean for two free fields of mass m with interactions $O(g)$. Linear combinations of these fields have z spin $l^z = \pm 1$. These excitations are normally referred to as spin waves. Naively, they become massless in the isotropic limit: $a, b, m \to 0$. In order to discuss explicitly the soliton solution it is convenient to adopt spherical coordinates: $\boldsymbol{\phi} = (\sin\rho\cos\beta, \sin\rho\sin\beta, \cos\rho)$. The time-independent soliton has $\beta = \text{const}$ and $\rho(x)$ varying from 0 to π. The dyon solution has $\beta = \omega t$. Thus β plays the role of the rigid-rotator collective coordinate introduced earlier. In terms of ρ and β the Lagrangean density becomes

$$L = (1/2g)[(\partial^\mu\rho\,\partial_\mu\rho + \sin^2\rho\,\partial^\mu\beta\,\partial_\mu\beta + m^2\cos^2\rho] + (\theta/4\pi)\epsilon^{\mu\nu}\partial_\mu(\cos\rho\,\partial_\nu\beta). \tag{6}$$

Setting $\beta = \text{const}$, we obtain the sine-Gordon Lagrangean with soliton solution: $\cos\rho = \tanh mx$. Its energy relative to the ground state is

$$E = (1/2g)\int dx[(\partial\rho/\partial x)^2 + m^2\sin^2\rho] = 2m/g. \tag{7}$$

To find the low-frequency dyon solutions we may set $\rho(x)$ equal to its value for the static soliton solution, substitute into L, and integrate over x, giving $L = (1/gm)(\dot\beta)^2 - (\theta/2\pi)\dot\beta$. We may take over the analysis of the rigid rotator given above with moment of inertia $I = 2/gm$. We conclude that the allowed dyon frequencies are $\omega = (gm/2)(n + \theta/2\pi)$ and the rotator energies are $E = (gm/4)(n + \theta/2\pi)^2$. This analysis is only valid for $gn \ll 1$ (i.e., $n \ll s$); there are terms in $L(\dot\beta)$ of higher order in $\dot\beta^2$ arising from both classical and quantum corrections. In terms of the original parameters, the dyon energy and precession frequency to lowest order in $1/s$ are

$$E_n = J[2(a+b)]^{1/2}\{s^2(1-\alpha^2) + 8[n + s(1+\alpha)]^2\} \tag{8}$$

and $\omega_n = J[2(a+b)]^{1/2}[n + s(1+\alpha)]$. The integer n in these formulas is the total z component of spin of an *even* number of sites containing the dyon. To see this note, if we sum over an even number of sites, that

$$S^z \equiv \sum_{2j}^{2k+1} S_i^z = \int dx\, l^z = \int dx\,\partial L/\partial\dot\beta = n. \tag{9}$$

If we consider a chain with an odd number of sites it necessarily contains a dyon. The total z spin is now $S^z = n + s$, the second term coming from the unpaired spin which we take to be far from the center of the dyon. Specializing to the case $\alpha = 0$, we see that the lowest-energy dyon state is a singlet with $S^z = 0$ for s integer but is a doublet with $S^z = \pm\frac{1}{2}$ for s half-integer. In either case all levels with $n \neq 0$ are doubly degenerate. As α is turned on these levels split with crossings occurring each time that $s\alpha$ passes through a half-integer or integer. Thus θ has an effect $O(1)$ on the dyon, although its effects are generally $O(e^{-\pi s})$. This is so because the topological term is $(1/4\pi)\dot\beta \times \int dx\, d(\cos\rho)/dx$. The integral is the soliton number and $\dot\beta$ is the z spin, both of which are nonzero for a dyon. They are analogous, respectively, to the magnetic and electric charge of the particle-physics dyon. It should be emphasized that although the above quantitative analysis is only valid in a very restricted range of parameters, the general phenomenon of splitting of dyon levels by a P-nonconserving interaction is much more general since it follows from symmetry considerations alone.

We now consider the prospects for experimental observation of this phenomenon. Crystals that approximate one-dimensional antiferromagnets well are known. An example with Ising anisotropy and $s = \frac{1}{2}$ is $CsCoCl_3$. A broad peak in the frequency-dependent susceptibility, indicative of solitons,[11] has been observed[12] in neutron scattering. Precessing solitons, dyons, have not yet, to my knowledge, been observed. For the above picture to be appropriate the spin would have to be reasonably large and the anisotropy quite small [the $s = \frac{5}{2}$ one-dimensional antiferromagnet $(CH_3)_4NMnCl_3$ shows behavior typical of the large-s limit and has a small anisotropy of about 1%; however, the anisotropy is planar rather than Ising]. On the assumption that such a material could be found, a possible method for detecting the dyon levels would be to excite transitions between them by neutron scattering. Supposing, for the moment, that $\alpha = 0$, it might be possible to excite transitions between dyon states of different S^z by a neutron scattering event in which the neutron spin flips and S^z changes by one unit. For half-integer s such a transition could occur between the degenerate soliton ground states; in the integer-s case some of the kinetic energy, $\Delta E \approx 8J[2(a+b)]^{1/2}$ in the above approximation, would be turned into internal dyon energy, associated with the precession. If $\alpha = 0$, the same energy shift would be observed for $\Delta S^z = \pm 1$ and for soliton or antisoliton. This should be the lowest energy and most probable process which changes S^z by ± 1. The massive spin waves discussed above have spin ± 1 and so their spin cannot change by one unit.

There is no indication of alternating interactions in $CsCoCl_3$ or $(CH_3)_4NMnCl_3$. However, such interactions, arising from the spin-Peierls effect, have been seen[8] in the quasi one-dimensional $s = \frac{1}{2}$ antiferromagnets $TTFXS_4C_4(CF_3)_4$, where $X = Cu$ or Au and TTF denotes tetrathiafulvalinium. The parameter α was observed to be 0.127 and 0.033, respectively. It is not clear that Ising anisotropy is compatible with the spin-Peierls effect which is a lattice instability induced by the massless antiferromagnetic phase. However, if a system could be found with these two types of asymmetry (the alternating interactions could arise from effects unconnected with magnetism) then it might be possible to observe the fractional shift in dyon levels from neutron scattering. For integer s, two different inelastic energy shifts would now be observed for $\Delta S^z = +1$ corresponding to scattering off a soliton or antisoliton. The difference between these energies is, in the above approximation, $\Delta E \approx 32J \times [2(a+b)]^{1/2} s\alpha$. A similar result holds for half-integer spin. It might also be possible to observe transitions between dyon levels by resonant adsorption of (microwave) photons. A useful way of disentangling the dyon levels might be the application of a magnetic field, h, in the z direction. This shifts the energy of a dyon of angular momentum S^z by $2\mu_B h S^z$ (where μ_B is the Bohr magneton), thus splitting the levels which are degenerate if $\alpha = 0$.

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