Spinon deconfinement above a finite energy gap in two-dimensional quantum Heisenberg antiferromagnets

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The familiar spin-$\frac{1}{2}$ quantum Heisenberg antiferromanget in a two-dimensional (2D) square lattice is shown, within the nonlinear sigma model approximations, to be another state of matter that has excitations with fractional quantum numbers above a finite energy gap. The 1-skyrmion with an energy $\approx 2\pi J$ is shown to be made of two "deconfined spinons" or "O(3) vortices." The many skyrmion operator and the wave functions that we have found are strikingly similar to quantum Hall quasiparticle operators and wave functions. We also predict the presence of finite energy "spin-S spinon" for a general spin S Heisenberg antiferromagnets in 2D. Some consequences are briefly discussed.

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Neutral spin-$\frac{1}{2}$ fermionic excitations,[1] now called "spinons"[2] were conjectured to be present in the quantum spin liquid states of spin-half two-dimensional (2D) Heisenberg antiferromagnets, by Anderson in 1987. While this was readily shown to be present in the resonating valence bond (RVB) mean-field analysis[3] of the spin liquid vacua and short-range RVB states,[4] their presence as a finite energy deconfined excitation in the ordered antiferromagnetic vacua has remained unclear.

A conjecture by Dzhyaloshinskii, Wiegman, and Polyakov[5] and the early work of Wilczek and Zee[5] suggested statistics transmutation of skyrmion in ordered spin-$\frac{1}{2}$ Heisenberg antiferromagnets in 2D. Anderson, John, Doucot, Liang, and the present author[6] however conjectured that finite energy "half-skyrmion" or "meron"[7] is the "deconfined" spinons based on some heuristic arguments.

Recent inelastic neutron-scattering results covering a large energy and momentum range in the insulating cuprates,[8] and also Raman[9] and infrared measurements, make the search for any signatures of spinons at low and high energies very meaningful and urgent.

The aim of the present paper is to study the spectrum of quantum Heisenberg antiferromagnet in 2D and look for deconfined spinons above a finite energy gap, within the O(3) nonlinear sigma (NLS) model approach. We look carefully at Belavin-Polyakov[10] n-skyrmion *static classical solutions*. The mathematical structure of the n-skyrmion solution in one particular parametrization readily suggests that each skyrmion is made of $2n$ constituent point particles.[7,11,12]

To understand the quantum dynamics of these constituent particles we construct the skyrmion operator for our spin-$\frac{1}{2}$ Heisenberg antiferromagnet and discover that the creation operator for these constituent particles has mathematical structure similar to Laughlin's quasihole and quasiparticle operators of quantum Hall effect. By a Berry phase analysis we show their spin to be half. Asymptotic form of the modulus of the n-skyrmion wave function in terms of collective coordinates is also found.

Our starting point is the spin-S quantum Heisenberg antiferromagnet in a 2D square lattice with nearest-neighbor interactions. Following the standard derivation[13] one arrives at the O(3) NLS model action along with the important lattice sum of Berry phases:

$$S=\frac{\rho_0}{2}\int dx\,dy\,dt\left([\boldsymbol{\partial}_\mu \mathbf{n}(\mathbf{r})]^2-\frac{1}{v_s^2}[\partial_t \mathbf{n}(\mathbf{r})]^2\right)+iS_B[\mathbf{n}]. \tag{1}$$

Here $\mu=x,y$ and $\mathbf{n}(\mathbf{r})$ is a normalized $[\mathbf{n}(\mathbf{r})\cdot\mathbf{n}(\mathbf{r})=1]$ sublattice magnetization vector.

The coefficient $\rho_0\approx J$ for $S=\frac{1}{2}$ case, and v_s is the spin wave velocity. The Berry phase term is a lattice sum:

$$S_B[\mathbf{n}]=2\pi S\sum_{m,n}(-1)^{|m|+|n|}\Omega^o(\mathbf{n}_{m,n}). \tag{2}$$

Here the integers (m,n) stand for a lattice site, and $\Omega^o(\mathbf{n}_{m,n})=\int dt\,du/8\pi\mathbf{n}_{m.n}\cdot(\partial_t\mathbf{n}_{m.n}\times\partial_u\mathbf{n}_{m.n})$ is the single-site Berry phase.

Inspired by the conjecture of Ref. 6 we look at the finite energy topological solutions in our search for spinons. The multiskyrmion solutions found by Belavin and Polyakov[10] are extended objects with nontrivial topology. Their Euclidean solutions of the O(3) model in (1+1)D become the time-independent classical solutions of our O(3) model in (2+1)D.

An n-skyrmion solution is given by

$$w(z)=\prod_{i=1}^{n}\left(\frac{z-a_i}{z-b_i}\right). \tag{3}$$

Here $z=x+iy$. The n complex coordinates a_i and b_i characterize the skyrmion solution. The function $w(z)$ and the sublattice magnetization $\mathbf{n}(\mathbf{r})\equiv[\sin\phi(\mathbf{r})\cos\theta(\mathbf{r}),\sin\phi(\mathbf{r})\sin\theta(\mathbf{r}),\cos\phi(\mathbf{r})]$ are related by

$$w(z)\equiv\cot\frac{\phi(\mathbf{r})}{2}e^{i\theta(\mathbf{r})}. \tag{4}$$

The n-antiskyrmion solutions are obtained by replacing z by $\bar{z}$. In our convention the spins at infinity $\mathbf{n}(\infty)=(1,0,0)$ for the ground as well as the skyrmion/antiskyrmion states, since $w(\infty)=1$.

The energy of the n-skyrmion solution is given by

$$E_{cl}^n=4\pi\rho_0 n, \tag{5}$$

a constant independent of the skyrmion coordinates $\{a_i, b_i\}$ This means that at the classical level the n-skyrmions do not interact; thus the set $\{a_i, b_i\}$ represents the $2n$ "zero-mode" (two-dimensionall) coordinates of the n-skyrmion. We will call a and b the coordinates of the $2n$ constituent particles of an n-skyrmion.

Physically the coordinates a and b represent the "centers" of local vortex distortions of the xy component of the three-vector field $\mathbf{n}$. However, unlike the $\pm$ vortex pair of an xy model, there is a freedom in the choice of the positions of the vortex pair; for a 1-skyrmion any two diametrically opposite points on the circle $|z-(a+b)/2| = |(a-b)/2|$ can be chosen as centers of the vortex pair, with the local vortex distortion occurring in appropriately rotated 2D plane in the spin space. It is remarkable that the extended spin twists of a 1-skyrmion, which are more of a "ringlike" distortion of the $\mathbf{n}$ field than two point vortices, are characterized by just two points a and b, which we will later elevate to the level of particle degrees of freedom in the plane. We say that an n-skyrmion is made of $2n$ "O(3) vortices."

It should be remarked that the Belavin-Polyakov exact solutions describe either skyrmions or antiskyrmions. No exact solution containing both skyrmions and antiskyrmions exists. In approximate solutions containing 1-skyrmion and 1-antiskyrmion there is a dipolelike interaction between them even at the classical level.[7]

The two O(3) vortices of a 1-skyrmion state are finite energy solutions and they have twisted their way out of the $\ln|a-b|$ energy dependence, characteristic of xy vortices in $2D$. We will see later that quantum fluctuations produce repulsion between the two O(3) vortices of a 1-skyrmion. Further, once an xy anisotropy is introduced the O(3) vortices degenerate to two xy vortices with an energy diverging as $(J_x - J_z)/J_z \ln|a-b|$ as $|a-b| \to \infty$.

An n-skyrmion/antiskyrmion carries a topological "quantum number" or a "winding number" $\pm n$, the degree of the map $(x,y) \to S^2$ of the field $\mathbf{n}(x,y)$. Here S^2 is the order parameter space. The "topological density" $q(\mathbf{r})$ is given by

$$q(\mathbf{r}) = \frac{1}{8\pi}\mathbf{n}(\mathbf{r}) \cdot [\partial_x \mathbf{n}(\mathbf{r}) \times \partial_y \mathbf{n}(\mathbf{r})] = \frac{[\partial_z w \partial_{\bar{z}} \bar{w} - \partial_{\bar{z}} w \partial_z \bar{w}]}{\pi(1+|w(z)|^2)^2}, \tag{6}$$

and $\int dx dy q(\mathbf{r}) = n$ is the winding number.

To keep comparison with other formalisms, the above topological density is related to the U(1) magnetic flux of the RVB gauge field:[14]

$$\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k) \equiv i(\tau_{ij}\tau_{jk}\tau_{ki} - \tau_{ik}\tau_{kj}\tau_{ji}) \sim e^{i\oint \mathbf{A}_{rvb} \cdot d\mathbf{l}}, \tag{7}$$

where $\tau_{ij} = \Sigma_\sigma c^\dagger_{i\sigma} c_{j\sigma}$ and $n_{i\uparrow} + n_{i\downarrow} = 1$.

To understand the quantum dynamics of the skyrmion excitation and its constituent particles for our spin-$\frac{1}{2}$ Heisenberg model on the square lattice, we first construct the operator for the 1-skyrmion on the lattice. (No exact classical solution is available for the "lattice version" of the NLS model in 2D; when $|a-b| \gg 1$, in units of the lattice parameter, the continuum skyrmion solution should be a good approximation to the lattice solution.) The spin-wave ground state of our spin-$\frac{1}{2}$ Heisenberg antiferromagnet is

$$\Psi_{sw}[z,\bar{z}] \sim (-1)^{N_A} \exp\left\{ -\sum_{i<j} f(|z_i - z_j|) \right\}, \tag{8}$$

where $z_i \equiv m_i + i n_i$ stands for the lattice coordinates of the $N_0/2$ down-spin electrons in the square lattice containing N_0 sites. This is a *hard-core boson* (or equivalently s^z) representation of the spin-wave ground state, where the Jastrow factor $f(|z_i - z_j|) \sim 1/|z_i - z_j|$ arises from the zero-point quantum fluctuations of the gapless spin-wave modes of the ordered antiferromagnet and $(-1)^{N_A}$ is the Marshall sign factor, where N_A counts the number of down spins on sublattice A. The off-diagonal long-range order exhibited by the above $N_0/2$ hard-core boson wave function represents the long-range antiferromagnetic order, with a finite sublattice magnetization $\mathbf{m}$, lying in the xy plane. We can fix the direction of $\mathbf{m}$ in the xy plane by giving an additional coherent superposition with respect to S^z_{total} (the total number of hard core bosons) in the above wave function.[15]

After some algebra the coordinate representation of the 1-skyrmion operator is shown to be

$$\hat{\mathbf{O}}^{(1)}_{Sk}(a,b) \equiv \prod_{i=1}^{N_0/2} \left(\frac{z_i - a}{z_i - b} \right). \tag{9}$$

While $w(z)$ of Eq. (3) represents the distortion of the sublattice magnetization in space, Eq. (9) provides the operator that produces the distortion. To prove the above, it is convenient to put the sublattice magnetization along the $+x$ axis in the ground state and use the s^z representation,

$$\hat{\mathbf{O}}^{(1)}_{Sk}(a,b) \equiv \Pi_{i=1}^{N_0} \left(\frac{z_i - a}{z_i - b} \right)^{s_i^z + 1/2}.$$

[Note, that unlike Eq. (9), here z_i's run over all sites.]

This is an important result, which shows that a 1-skyrmion operator actually creates one Laughlin[16] quasihole and one quasielectron-like object, when acting on the hard-core Bose fluid. Similarly an n-skyrmion state can be created by a product of n of Laughlin quasiholes and n of quasi-electron-like operators. The operator for antiskyrmion is obtained by replacing $\{z_i\}$ by $\{\bar{z}_i\}$ in Eq. (9). Our quasihole operator exactly coincides with Kalmayer-Laughlin spinon operator.[16]

Since at the classical level, the a and b coordinates of the n-skyrmion solution represent the zero-mode coordinates, it is legitimate to elevate them to the level of new low-energy collective coordinates or "particle degrees of freedom,"[12] as in the case of Laughlin's quasiholes and quasielectrons.

While the a and b "quasiparticles" [O(3) vortices] do not have any interaction at a classical level, the modified quantum fluctuations in the presence of a skyrmion can induce interactions among the constituent particles. The induced interaction $V_{qu}(a,b)$ is obtained from the difference in zero-point energy of the spin-wave modes in the presence $\hbar\omega^{(a,b)}_\mu$ and absence $\hbar\omega^0_\alpha$ of a 1-skyrmion:

$$V_{qu}(a,b) \equiv \frac{1}{2} \sum_{\mu} \hbar \omega_{\mu}^{(a,b)} - \frac{1}{2} \sum_{\alpha} \hbar \omega_{\alpha}^{0}. \tag{10}$$

Using the method of Rodriguez[17]and also Marino,[18] who did not use the constituent particle interpretation, we have calculated the induced interaction between an a and b particles. We find that the a and b particles always repel. It is energetically advantageous for the constituent particles to be infinitely apart and reduce the zero-point fluctuation energy. In particular the quantum fluctuation corrected energy of a 1-skyrmion state is

$$E_{qu}^{n=1}(|a-b| \to 0) \approx 4\pi J,$$

$$E_{qu}^{n=1}(|a-b| \to \infty) \approx 2\pi J.$$

This proves that the two constituent particles are indeed deconfined.

I have obtained an asymptotically exact *modulus of the wave function* of the ground state of the n-skyrmion state, for large separation of the a and b coordinates as

$$|\Psi_n[a,b]| \sim \prod_{i<j} |a_i - a_j||b_i - b_j| \prod_{i,j} |a_i - b_j|^{-1}. \tag{11}$$

The method I have devised involves expressing the path integral for vacuum to vacuum amplitude in a way that gives the desired wave function in terms of the Jacobian of transformation from the function $w(z)$ to the zero-mode coordinates. A plasma analogy shows that the a and b particles are indeed unbound, giving another proof for the deconfinement of the a and b particles in the skyrmion state.

The spin of a skyrmion or the constituent O(3) vortices and their exchange statistics are rather ill defined in view of the large quantum fluctuation contained in the spin-wave ground state. The ''mathematically sharp'' point particles a and b are extended physical objects with power-law form factors. (This is similar to the case[19] of vortices in 2D superfluid ^{4}He). The integrated missing or excess density around a vortex gives the z component of the spin of the a and b particles. This calculation turns out to be hard with our hard-core Bose fluid. So we take a Berry phase approach.

In our Berry phase analysis the spin of the constituent particle or the O(3) vortices appears as a ''chain anomaly.'' We consider a 1-skyrmion solution and analyze the lattice sum of the Berry phases under a global rotation of all the spins through 2π about x axis, the direction of sublattice magnetization at infinity. If the spin projections of the constituent particle along the x axis are σ_a and σ_b, the corresponding lattice sum of Berry phases should contribute $2\pi\sigma_a$ and $2\pi\sigma_b$ for the a and b particles in a spatially separated fashion.

We find an interesting phenomenon which we call a chain anomaly. We group, following Haldane,[13] the square lattice sum of Berry phases into sums over chains, running parallel to the x axis:

$$S_B = 2\pi S \sum_{n} (-1)^n \Omega_n^{1d}, \tag{12}$$

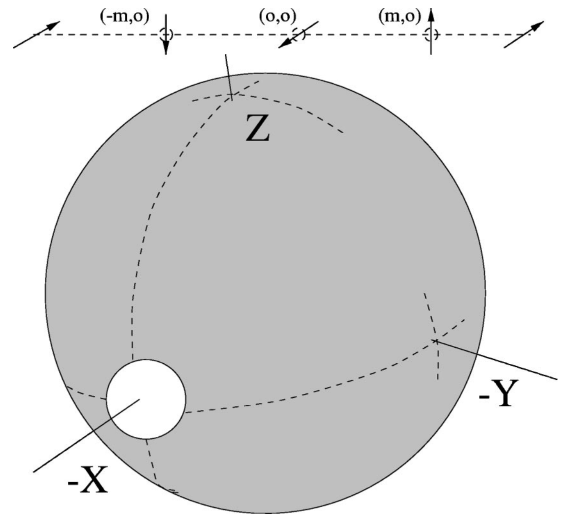

FIG. 1. The ''hole'' in S^2 of the map $(x,t) \to S^2$ of the field $\mathbf{n}(x,n;t)$ for a $n \neq 0$ chain. The hole just vanishes for the $n=0$ chain; inset shows its $\mathbf{n}(x,0;t)$ at $t=0$.

where the nth chain Berry phase is given by the sum

$$\Omega_n^{1d} \equiv \sum_{m=-N,\ldots,N-1} (-)^m \Omega^o(\mathbf{n}_{m,n})$$

$$= \int \frac{dx dt}{8\pi} \mathbf{n}(x,n;t) \cdot [\partial_x \mathbf{n}(x,n;t) \times \partial_t \mathbf{n}(x,n;t)]. \tag{13}$$

The chain Berry phase counts the winding number of map $(x,t) \to S^2$ of the field $\mathbf{n}(x,n;t)$ for nth chain.

We choose the length of our lattice along the x axis to be $2N$, where N is an odd integer. For convenience we choose (0,0) to be the center of the square lattice and the two skyrmion coordinates to be the lattice sites, $a=(m,o)$ and $b=(-m,0)$ on the x axis at time $t=0$ and T. Our global rotation amounts to giving the following time dependence $a(t)=me^{i2\pi t/T}$ and $b(t)=-me^{i2\pi t/T}$ to the constituent particle coordinates.

During the time evolution, the spin field $\mathbf{n}(x,n;t)$ of the 1-skyrmion state of any chain n attempts to wrap the S^2 sphere. All, except the x-axis chain $(n=0)$, fail to wrap the S^2 sphere completely. They all leave a hole, as shown in Fig. 1, making the winding number (Berry phase) identically zero. The x axis chain just manages to wrap the S^2 sphere, once for the chain sum $-N,\ldots,-1$ and again in the opposite sense for the chain sum $0,1,\ldots,N-1$, thereby contributing a phase of π for the left half and $-\pi$ for the right half of the chain. We identify these two phases, which arise predominantly from the a-vortex region and b-vortex region, with the spin-$\frac{1}{2}$ Berry phases of a and b particles.

The lattice sum of Berry phases can be grouped in many different ways and *we always find one singular chain* passing through two diametrically opposite points of the circle $|z-a+b/2|=|a-b/2|$, of our 1-skyrmion solution. The two ends of the chain either close on themselves or go off to infinity. The spin field $\mathbf{n}$ for these singular chains traces a closed curve in S^2 connecting two antipodal points at any given time; *it undergoes "π-twist" twice, corresponding to the presence of two spinons*. For example, the circle $|z-a+b/2|=|a-b/2|$ itself is a singular chain, for which the **n** field traces a great circle on S^2 at any given time.

In spin-$\frac{1}{2}$ Heisenberg chain each π *twist* of **n** field in space corresponds to one spinon.[20] In a sense, *in the 1-skyrmion configuration a "1D-chain" or a "string" containing two spinons is embedded in the 2D plane in an irreducible and degenerate fashion*.

Our chain anomaly is missed if we use Haldane's argument[13] for the calculation of the Berry phase. Haldane suggested that if the $\mathbf{n}(x,y;t)$ field is continuous and nonsingular (as it is for the case for *n*-skyrmion solution), the chain Berry phases should be all identical and as a result the staggered sum should be identically zero, for an even number of chains. However, we find that our singular chain containing the a and b coordinate is an exception to this and it contributes a Berry phase of π and $-\pi$ to the two particles a and b.

The two O(3) vortices or the two spinons of a 1-skyrmion state, by the argument given above, carry spin half projections of value $\frac{1}{2}$ and $-\frac{1}{2}$ along the x axis. In addition the spinons carry $+1$ chirality quantum number because they are constituent particles of a + 1-skyrmion state. Thus a spinon in addition to a spin quantum number carries a ± 1 chirality quantum number. As the antiferromagnetically ordered ground state has zero chirality, the finite energy skyrmion states are chiral doublets. It should be interesting to look for this degeneracy in the excited states in numerical studies of finite systems. This degeneracy is also reminiscent of the degeneracy of the spinon states in the 1D Haldane-Shastry model arising from the Yangian symmetry.

Our analysis goes through for any spin. In general for the spin-S square lattice Heisenberg model we get deconfined spin-S spinons or the O(3) vortices.

The spinon deconfinement that we have found has several interesting consequences which we hope to discuss in the future: (i) suggests a way to produce charge $2e$ skyrmions to get superconductivity in the doped Mott insulator, (ii) as the energy of a deconfined spinon $\approx \pi J$, its possible signature at the top of the spin-wave band as well as in the infrared and two magnon Raman measurements, (iii) short-range RVB state viewed as the condensation of skyrmion and antiskyrmion in the ground state; chiral symmetry broken Kalmayer-Laughlin-like states as condensation of unequal density of skyrmion and antiskyrmion, and (iv) consequence of our present picture to skyrmion doping in quantum Hall ferromagnets.

Our identification of O(3) vortices as spinons and their deconfinement in an ordered antiferromagnet is a non-trivial result. This is missed in approximate treatments,[21] where certain U(1) vortices are identified with spinons, which are confined by linear potential in the ordered phase.

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