Pairing of Solitons in Two-Dimensional $S = 1$ Magnets

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We study a general model of isotropic two-dimensional spin-1 magnet, which is relevant for the physics of ultracold atoms with hyperfine $S = 1$ spins in an optical lattice at odd filling. We demonstrate a novel mechanism of soliton pairing occurring in the vicinity of a special point with an enhanced $SU(3)$ symmetry: upon perturbing the $SU(3)$ symmetry, solitons with odd CP^2 topological charge are confined into pairs that remain stable objects.

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Introduction.—Many condensed matter systems can be successfully described with the help of low-energy effective continuum field models. In systems with reduced spatial dimensionality, topologically nontrivial field configurations (solitons) are known to play an important role [1]. In many magnetic systems the fluctuations of the magnetization length occur at a higher energy scale and can be neglected. The effective theory is then the so-called $O(3)$ nonlinear sigma model (NLSM), and its topological excitations are well understood [2].

One has to go beyond the NLSM description in case of proximity to quantum phase transitions. Our interest is in the general $S = 1$ model on a two-dimensional (2D) square lattice described by the Hamiltonian

$$\mathcal{H} = \sum_{\langle ij\rangle} h_{ij}, \qquad h_{ij} = -J(\boldsymbol{S}_i \cdot \boldsymbol{S}_j) - K(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2, \quad (1)$$

where $\langle ij\rangle$ denotes the sum over nearest neighbors, and J and $K > 0$ are, respectively, the bilinear (Heisenberg) and biquadratic exchange constants. This model describes physics of ultracold alkali atoms with hyperfine $S = 1$ spins (e.g., ^{23}Na) in optical lattices at odd filling [3], and parameters J and K can be varied by tuning the ratio a_2/a_0 of scattering lengths in $S = 2$ and $S = 0$ channels using the Feshbach resonance. Similar models were proposed [4] as a possible explanation for the unconventional spin state discovered recently [5] in the quasi-2D $S = 1$ magnet $NiGa_2S_4$, and were also discussed [6] in context of the deconfined quantum criticality conjecture [7].

The model (1) has $SU(2)$ symmetry that is enlarged to $SU(3)$ at two points, $J = K$ and $J = 0$. The point $J = K$, which marks the ferromagnetic-ferroquadrupolar transition, corresponds to $a_2 = a_0$ [3] in the cold bosons case with one atom per site. Our goal here is to show that the crossover from $SU(3)$ to $SU(2)$ symmetry features a novel mechanism of topological pairing: solitons with odd CP^2 topological charge are confined into stable pairs. This is in contrast to the usual scenario where solitons collapse if the symmetry is lowered [e.g., $U(1)$ vortices when $U(1)$ gets broken down to Z_2].

Continuum field description.—The spin-1 state $|\psi\rangle_j$ at a given site j is a linear superposition of three basis states $|\sigma\rangle_j$ with $S_j^z|\sigma\rangle_j = \sigma|\sigma\rangle_j$, $\sigma = 0, \pm 1$. It is convenient to write down the spin-1 state at site j as

$$|\psi\rangle_j = \sum_{a=x,y,z} t_{j,a}|a\rangle_j, \quad (2)$$

using the "Cartesian" states $|z\rangle = |0\rangle$, $|x\rangle = (|-1\rangle - |+1\rangle)/\sqrt{2}$, $|y\rangle = i(|-1\rangle + |+1\rangle)/\sqrt{2}$, then the three numbers t_{ja} transform under rotations as the components of a complex vector $\boldsymbol{t}_j$, with the normalization $\boldsymbol{t}_j^* \cdot \boldsymbol{t}_j = 1$. The states (2) can be viewed as $SU(3)$ coherent states corresponding to the bosonic operators $\hat{t}_{j,a}$, and the $S = 1$ operator can be represented as $S_j^a = -i\epsilon_{abc}\hat{t}^\dagger_{j,b}\hat{t}_{j,c}$. Since the overall phase factor in (2) can be arbitrary, the order parameter space of the problem is isomorphic to CP^2.

The lattice Lagrangian of the model expressed in terms of the complex unit vector $\boldsymbol{t}$ takes the form

$$\mathcal{L} = \sum_j i(\boldsymbol{t}_j^* \cdot \partial_t \boldsymbol{t}_j) - W, \qquad W = \sum_{\langle ij\rangle} \langle \hat{h}_{i,j}\rangle, \quad (3)$$

where the local Hamiltonian average $\langle \hat{h}_{i,j}\rangle$ is given by

$$\langle \hat{h}_{i,j}\rangle = J(\boldsymbol{t}_i^* \cdot \boldsymbol{t}_j)(\boldsymbol{t}_j^* \cdot \boldsymbol{t}_i) + (J - K)(\boldsymbol{t}_i^* \cdot \boldsymbol{t}_j^*)(\boldsymbol{t}_i \cdot \boldsymbol{t}_j). \quad (4)$$

The Lagrangian is invariant under global rotations $t_{j,a} \mapsto \mathcal{R}_{ab}t_{j,b}$, with an arbitrary $O(3)$ rotation matrix $\mathcal{R}$, as well as under local "gauge" transformation $\boldsymbol{t}_j \mapsto \boldsymbol{t}_j e^{i\chi_j}$. At $J = K$ the symmetry becomes higher as there is an invariance under a global transformation $\boldsymbol{t}_j \mapsto U\boldsymbol{t}_j$, with $U \in SU(3)$. If the lattice is bipartite, at $J = 0$ the energy is invariant under an arbitrary $SU(3)$ rotation on the sites belonging to one sublattice, accompanied by a conjugate transformation $\boldsymbol{t}_j \mapsto U^*\boldsymbol{t}_j$ at the other sublattice, so the point $J = 0$ is $SU(3)$ invariant as well.

Breaking up the complex vector $\boldsymbol{t} = \boldsymbol{u} + i\boldsymbol{v}$ into two real vectors representing its real and imaginary parts, one can write the on-site spin and quadrupole averages as

$$\langle \boldsymbol{S} \rangle = 2(\boldsymbol{u} \times \boldsymbol{v}),$$
$$S_{ab} \equiv \langle S_a S_b + S_b S_a \rangle = 2(\delta_{ab} - u_a u_b - v_a v_b). \quad (5)$$

One can use a different parametrization, directly connected to the physical averages, by introducing the eight-component vector $\boldsymbol{n}$,

$$n_\alpha = \boldsymbol{t}^* \cdot \hat{\lambda}_\alpha \boldsymbol{t}, \quad (6)$$

where $\hat{\lambda}_\alpha$, $\alpha = 1, \ldots, 8$, are the well-known Gell-Mann matrices that form, together with a unit matrix $\mathbb{1}$, a basis in the $SU(3)$ matrix space. The vector $\boldsymbol{n}$ is subject to the following two constraints:

$$\boldsymbol{n}^2 = 4/3, \qquad \boldsymbol{n} \cdot (\boldsymbol{n} * \boldsymbol{n}) = 8/(3\sqrt{3}), \quad (7)$$

where the $*$ product of any two vectors $\boldsymbol{n}$ and $\boldsymbol{n}'$ is defined as $(\boldsymbol{n} * \boldsymbol{n}')_\alpha = \sqrt{3} d_{\alpha\beta\gamma} n_\beta n'_\gamma$, and $d_{\alpha\beta\gamma}$ are the structure constants defined by the anticommutation properties of the Gell-Mann matrices, $\{\lambda_\alpha, \lambda_\beta\} = \frac{4}{3}\delta_{\alpha\beta}\mathbb{1} + 2d_{\alpha\beta\gamma}\lambda_\gamma$. One can show that the constraints (7) in fact reduce the dimension of the $\boldsymbol{n}$ space to four. The quantities n_α correspond to the following on-site averages:

$$n_2 = \langle S_z \rangle, \qquad n_5 = -\langle S_y \rangle, \qquad n_7 = \langle S_x \rangle,$$
$$n_4 = S_{xz}, \qquad n_6 = S_{yz}, \qquad n_1 = S_{xy}, \quad (8)$$
$$n_3 = (S_{xx} - S_{yy})/2, \qquad n_8 = \sqrt{3}(S_{zz}/2 - 2/3),$$

which can be split into the vector of spin averages $\boldsymbol{m}$ and the vector of quadrupolar averages $\boldsymbol{d}$,

$$\boldsymbol{m} = (n_7, -n_5, n_2), \qquad \boldsymbol{d} = (n_1, n_3, n_4, n_6, n_8). \quad (9)$$

In those variables, the Hamiltonian takes the simple form

$$\langle h_{i,j} \rangle = -\frac{K}{3} - \frac{K}{2}(\boldsymbol{d}_i \cdot \boldsymbol{d}_j) + \frac{1}{2}(K - 2J)(\boldsymbol{m}_i \cdot \boldsymbol{m}_j), \quad (10)$$

which explicitly shows that $J > K$ corresponds to a ferromagnet (FM), $J < 0$ to an antiferromagnet (AFM), and $0 < J < K$ to a quadrupolar (spin nematic) order (hereafter we assume that $K > 0$ and will not discuss the so-called orthogonal spin nematic present at $K < 0$).

In terms of $\boldsymbol{n}$, the lattice Lagrangian can be written as $\mathcal{L} = \sum_j \Phi(\boldsymbol{n}_j) - \sum_{\langle ij \rangle} \langle h_{ij} \rangle$, with the dynamic part

$$\Phi(\boldsymbol{n}) = \frac{3}{4} \frac{\boldsymbol{n}_0 \cdot (\boldsymbol{n} \wedge \partial_t \boldsymbol{n})}{1 + \frac{3}{2}\boldsymbol{n}_0 \cdot \boldsymbol{n}}. \quad (11)$$

Here the $SU(3)$ cross product is defined as $(\boldsymbol{n} \wedge \boldsymbol{n}')_\alpha = f_{\alpha\beta\gamma} n_\beta n'_\gamma$, where $f_{\alpha\beta\gamma}$ is another set of structure constants defined by commutators of the group generators $[\lambda_\alpha, \lambda_\beta] = 2i f_{\alpha\beta\gamma}\lambda_\gamma$, and $\boldsymbol{n}_0$ is an arbitrary vector satisfying the constraints (7).

Topological analysis.—To describe topological solitons, one needs to pass to the continuum description first. The continuum Lagrangian of the model (3) can be obtained by the gradient expansion of the discrete energy W retaining the leading terms that gives $W = \int d^2 x w$ with

$$w = J\{|\partial_\mu \boldsymbol{t}|^2 - |\boldsymbol{t}^* \cdot \partial_\mu \boldsymbol{t}|^2\} + (J - K)|\boldsymbol{t}^2|^2$$
$$- (J - K)\left\{|\boldsymbol{t} \cdot \partial_\mu \boldsymbol{t}|^2 + \frac{1}{2}[\boldsymbol{t}^2(\partial_\mu \boldsymbol{t})^2 + \text{c.c.}]\right\}, \quad (12)$$

where μ runs over space coordinates (x, y). The above form is valid for the region $J > K/2$, where the short-range spin-spin correlations are of the ferromagnetic type, as can be seen from (10).

To classify the topological excitations, one needs to know the so-called degeneracy space $\mathbb{M}_D$ that includes all values of the order parameter field corresponding to the ground state of the system. For the model (1) the space $\mathbb{M}_D$ is continuous and depends on the type of the ground state: for FM or AFM it coincides with the unit sphere S^2, for the nematic case it is a 2D real projective space $\mathrm{RP}^2 = S^2/Z^2$ (a unit sphere with the opposite points identified), and at $J = K$ the degeneracy space is enlarged to CP^2. For all the above spaces, the second homotopy group is nontrivial, $\pi_2(\mathbb{M}_D) = \mathbb{Z}$, which makes possible the existence of so-called localized topological solitons, whose order parameter distribution becomes uniform away from some point.

If the order parameter lies completely in $\mathbb{M}_D$, the energy contains only terms with gradients, so there is no natural space scale. If corresponding soliton solutions exist, they have a finite energy that does not depend on their size, and are stable against collapse. Another possibility is to allow the order parameter to leave $\mathbb{M}_D$, which breaks the scale invariance. Static solitons of that type are unstable against collapse due to the Hobart-Derrick theorem, but they can be stabilized by some internal dynamics [1,2]. We will study the structure of both types of solitons for the model (1).

For the sake of analyzing static soliton solutions, the Lagrangian (3) with the energy (12) is equivalent to the 2D CP^2 model [8] with an additional "anisotropy term" proportional to $(J - K)$. Let us start from the $SU(3)$-symmetric point $J = K$. In that case a localized topological soliton corresponds to the field configuration with nonzero topological charge [8]:

$$q = -\frac{i}{2\pi} \int d^2 x \epsilon_{\mu\nu} (\partial_\mu \boldsymbol{t}^* \cdot \partial_\nu \boldsymbol{t}), \quad (13)$$

where the indices μ, ν run over (x, y). The invariant (13) takes only integer values and corresponds to the mapping of the compactified 2D space S^2 onto CP^2. The exact $q = 1$ soliton solution is well known [8]:

$$\boldsymbol{t} = (\xi \boldsymbol{a} + z \boldsymbol{b})/\sqrt{|z|^2 + \xi^2}, \quad (14)$$

where $z = x + iy$ is the complex coordinate (the soliton center is assumed to be at the origin), $\boldsymbol{a}$ and $\boldsymbol{b}$ are two mutually orthonormal complex vectors, and ξ has the meaning of the soliton size. The energy of such excitation according to (12) is $E = 2\pi K$. For an arbitrary value of q, the general soliton solution can be written as

$$t_a = \frac{f_a}{(\sum_a |f_a|^2)^{1/2}}, \qquad f_a = c_a \prod_{k=1}^{q} (z - z_{k,a}), \qquad a = x, y, z, \tag{15}$$

and the corresponding energy is $E = 2\pi K|q|$.

Ferromagnetic solitons.—On the ferromagnetic side $J > K$ the minimum of energy is achieved for

$$\boldsymbol{t} = (\boldsymbol{e}_1 + i\boldsymbol{e}_2)/\sqrt{2} \tag{16}$$

with $\boldsymbol{e}_{1,2}$ being a pair of orthogonal real unit vectors. In that case, on the degeneracy space $\mathbb{M}_D$ the order parameter is equivalent to the unit vector $\boldsymbol{m} = (\boldsymbol{e}_1 \times \boldsymbol{e}_2)$ (a rotation around $\boldsymbol{m}$ corresponds to a change of the overall phase factor $\boldsymbol{t} \mapsto \boldsymbol{t}e^{i\varphi}$ and thus does not change the physical state). Thus, localized topological solitons for $J > K$ correspond to the mapping $S^2 \mapsto S^2$ and are characterized by another topological charge

$$Q_m = \frac{1}{8\pi} \int d^2x \varepsilon_{\mu\nu} \boldsymbol{m} \cdot (\partial_\mu \boldsymbol{m} \times \partial_\nu \boldsymbol{m}). \tag{17}$$

It is easy to calculate the topological charge (13) for a restricted field configuration satisfying (16): a general pair of orthonormal vectors $\boldsymbol{e}_{1,2}$ can be obtained from $\boldsymbol{e}_{x,y}$ by an arbitrary rotation $\mathcal{R}(\theta, \varphi, \psi)$, where θ and φ are, respectively, the polar and azimuthal angles characterizing the direction of the unit magnetization vector $\boldsymbol{m}$, and the third angle ψ corresponds to the rotation around $\boldsymbol{m}$. A straightforward calculation yields

$$q = \frac{1}{2\pi} \int d^2x \sin\theta \epsilon_{\mu\nu} (\partial_\mu \theta)(\partial_\nu \varphi) = 2Q_m. \tag{18}$$

One is led to conclude that solitons of the CP^2 model tend to pair upon perturbing the $SU(3)$ symmetry, which constitutes the central observation of this Letter.

The above result can also be obtained by noticing that for the configurations (16) the energy takes the form $W = (J/2) \int d^2x (\partial_\mu \boldsymbol{m})^2$. This is exactly the energy of the $O(3)$ NLSM, and the well-known Belavin-Polyakov (BP) soliton solution [9] with the topological charge $Q_m = 1$ will have the energy $E = 4\pi J$, which in the limit $J \to K$ is twice the energy of the $q = 1$ soliton (14) of the CP^2 model. In fact, one can explicitly check that the ferromagnetic BP soliton is a particular case of the general solution (14) with $q = 2$.

Solitons for spin nematic.—On the nematic side $J < K$ the minimum of energy is reached for $\boldsymbol{t} = \boldsymbol{u}e^{i\chi}$, where $\boldsymbol{u}$ is a real unit vector and χ is an arbitrary phase. The degeneracy space is thus $\mathbb{M}_D = \mathrm{RP}^2$. The energy then takes the form $W = K \int d^2x (\partial_\mu \boldsymbol{u})^2$, where $\boldsymbol{u}$ must be understood as a director; i.e., $\boldsymbol{u}$ and $-\boldsymbol{u}$ are identical. It is worth noting that in contrast to the other phases the spin nematic allows for a nontrivial π_1-topological charge as well, $\pi_1(\mathrm{RP}^2) = Z_2$.

If one defines the topological charge Q_u according to (17), simply replacing $\boldsymbol{m}$ by $\boldsymbol{u}$, then in the BP soliton with $Q_u = 1$ the director $\boldsymbol{u}$ goes over $\mathbb{M}_D$ twice; the energy of such a solution is $E_{\mathrm{BP}} = 8\pi J$. However, the director property of $\boldsymbol{u}$ allows one to construct a solution [10] with $\boldsymbol{u}$ going over $\mathbb{M}_D$ just once, which has $Q_u = \frac{1}{2}$ and the energy $\tilde{E}_{\mathrm{BP}} = 4\pi J$. In the limit $J \to K$ this is again twice as much as the energy of the $q = 1$ solution (14), which suggests that this soliton is a descendant of the $q = 2$ solution of the CP^2 model. This indicates that the tendency to pairing exists on the nematic side as well.

The fate of solitons with $q = 1$.—Up to now we have considered only static solitons with the order parameter lying completely inside $\mathbb{M}_D$. We found that for $J - K \neq 0$ the lowest energy solutions of that type are descendants of the $q = 2$ soliton of the CP^2 model, while the $q = 1$ solution seems to exist only at $J = K$. To get further understanding of what happens in the vicinity of the $SU(3)$-symmetric point $J = K$, let us discuss the CP^2 soliton with $q = 1$ for small but finite $J - K$. One can easily see that at $J - K \neq 0$ any solutions with $q = 1$ must involve a deviation of the order parameter from the degeneracy space $\mathbb{M}_D$. Because of the Hobart-Derrick theorem, this means instability of static solitons with $q = 1$ against collapse. However, $q = 1$ solitons can be stabilized by internal dynamics in the presence of additional integrals of motion; e.g., stable solitons with the magnetization vector precessing around the easy axis exist in the uniaxial ferromagnet [2]. In our case, it is also possible to construct such a solution. In terms of the complex vector $\boldsymbol{t} = \boldsymbol{u} + i\boldsymbol{v}$ this is a planar configuration, where $\boldsymbol{u}$ and $\boldsymbol{v}$ are parallel to the plane (1, 2) orthogonal to some axis $\boldsymbol{e}_3$; for definiteness let it be the z axis (a more general solution can be obtained by an arbitrary rotation). It is convenient to use the 8-vector notation (6): only four components of $\boldsymbol{n}$ are nonzero and it takes the form $\boldsymbol{n} = (R_x, R_z, R_y, 0, 0, 0, 0, 1/\sqrt{3})$, where $\boldsymbol{R}$ is a unit vector combining one spin average $R_z = m_3$ and two quadrupolar variables $R_x = d_1$, $R_y = d_2$ [cf. (9)]. Using (10) and (11), one obtains the effective Lagrangian for the chosen subspace,

$$\begin{aligned} \mathcal{L}_R &= \frac{1}{2} \sum_j \frac{\boldsymbol{R}_0 \cdot (\boldsymbol{R}_j \times \partial_t \boldsymbol{R}_j)}{1 + \boldsymbol{R}_0 \cdot \boldsymbol{R}_j} - W_R, \\ W_R &= -\sum_{\langle ij \rangle} \left[\frac{K}{2} \boldsymbol{R}_i \boldsymbol{R}_j + (J - K) R_{z,i} R_{z,j} \right], \end{aligned} \tag{19}$$

where $\boldsymbol{R}_0 = (0, 0, -1)$, and in (11) we have used $\boldsymbol{n}_0 = (0, 0, -1, 0, 0, 0, 0, \frac{1}{\sqrt{3}})$. The Lagrangian (19) describes the dynamics of a classical anisotropic ferromagnet with the unit magnetization vector $\boldsymbol{R}$; the anisotropy constant is proportional to $J - K$. At the isotropic point $J = K$ the energy $W_R = (K/2) \int (\nabla \boldsymbol{R})^2 d^2x$, and there exists a BP-type soliton that has the energy $E_{J=K} = 2\pi K$ and is a special case of the $q = 1$ CP^2 solution (14). The CP^2 charge q given by (13) is obviously equal to the Pontryagin index Q_R defined by (17) with $\boldsymbol{m} \mapsto \boldsymbol{R}$; the BP solution corresponds to the mapping of S^2 onto the subspace CP^1 embedded into CP^2 and has $Q_R = q = 1$.

For a finite "anisotropy" $(J - K)$ the BP soliton becomes unstable against collapse, but the situation is differ-

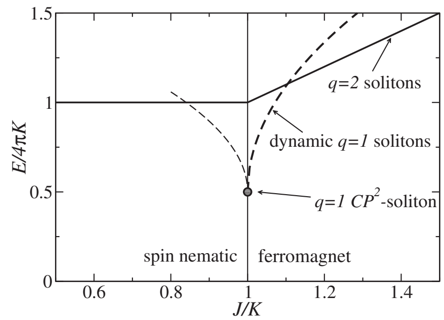

FIG. 1. Energy of topological solitons in the vicinity of the $SU(3)$-symmetric point $J = K$. Solid lines show the energy of static solitons with the CP^2 topological charge $q = 2$, and the dashed line corresponds to the descendants of the $q = 1$ soliton of the CP^2 model.

ent for the spin-nematic and FM regions. In the FM case ($J > K$) the anisotropy is of the easy-axis type, and there exist $Q_R = q = 1$ dynamic solutions, with $\boldsymbol{R}$ precessing around the z axis [2], which are smoothly connected to the BP solitons in the $J \to K$ limit. A detailed analysis [11] shows that the minimal energy of such dynamic solitons exhibits a nonanalytic behavior of the type $E_{\min} = E_{J=K}(1 + 3.74\sqrt{J/K - 1})$, as shown in Fig. 1. For small $J - K \leq 0.1K$, when the above expression is valid, the energy of a static $q = 2$ ($Q_m = 1$) soliton considered above stays higher than that of the $q = 1$ ($Q_R = 1$) dynamical soliton, but at the same time remains smaller than the energy of two dynamical $q = 1$ solitons, which indicates that it is energetically favorable to bind two $Q_R = 1$ solitons into a single $Q_m = 1$ one.

In the nematic case ($J < K$) we effectively have a ferromagnet with the easy-plane anisotropy. For such case, delocalized π_1 solitons (vortices) exist. Vortices in $\boldsymbol{R}$ field correspond to spin-nematic disclinations considered in Ref. [12]. The energy of a single vortex diverges logarithmically with the system size, so a static vortex-antivortex pair is unstable against collapse. The BP soliton can be considered as a pair of "merons" carrying topological charge $Q_R = \frac{1}{2}$ each [13]. For small $(K - J)$ those merons can be viewed as a vortex and antivortex with a finite out-of-plane component of the vector $\boldsymbol{R}$, they are subject to a gyroforce [12], and there may exist stable dynamic solutions (rotational pairs of vortices) similar to those studied in Refs. [14,15]. Their energy will tend to $2\pi K$ in the limit $J \to K$; similar to the FM case, in the vicinity of the $J = K$ point the $Q_R = 1$ topological solitons will be unstable against pairing into "nematic" Belavin-Polyakov solitons with $Q_u = \frac{1}{2}$.

Finally, a few words are to be said about the other, antiferromagnetic $SU(3)$–symmetric point $J = 0$. From (4) one can see that on any bipartite lattice the transformation $\boldsymbol{t}_j \mapsto \boldsymbol{t}_j^*$ for all j belonging to one sublattice maps the points $J = 0$ and $J = K$ onto each other. As can be seen from (10), and is especially clear from the "classical spin analogy" (19), for $J < K/2$ the short-range correlations are antiferromagnetic, and the proper transition to the continuum description becomes more complicated; however, one can show that the difference concerns only dynamics and does not affect the static properties. The arguments leading to (18) and thus the conclusion on soliton pairing equally apply to the vicinity of the $J = 0$ point.

Summary.—For a general non-Heisenberg model of the 2D isotropic $S = 1$ magnet, we have shown that in the vicinity of $SU(3)$-symmetric points topologically charged soliton excitations exhibit a peculiar topological pairing: in contrast to the usual scenario of soliton collapse with lowering the symmetry, solitons with odd CP^2 topological charge become confined into stable pairs when the $SU(3)$ symmetry is broken down to $SU(2)$.

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