New skyrmions in the attractive Hubbard model with broken SO(4) symmetry

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Abstract

The coexistence of superconducting and charge-density-wave order in the half-filled attractive Hubbard model is interpreted as a consequence of the pseudospin SU(2) symmetry spontaneously broken to a ‘hidden’ subgroup U(1). By topological arguments we show that there must exist new skyrmion textures associated with this symmetry breakdown. This fact is illustrated via a non-linear $\sigma$-model. Unlike the spin textures previously known in an antiferromagnetic background, doping the model away from half-filling leads the new skyrmions to unwrap.

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Recently, the Hubbard model has been a subject of intense study for its possible applications to high $T_c$ superconductivity [1]. It represents the simplest theoretical framework for describing strongly correlated electron systems. Despite its simple appearance, it is however quite difficult to analyze beyond one dimension. The elimination of phonon or other internal degrees of freedom can give rise to an effective attraction between the remaining electrons [2]. In this paper, we shall restrict ourselves to the Hubbard model of attractive interaction, which has been frequently applied to such compounds as bismuth oxide superconductors [3] and many others [4]. Numerical studies [5] showed that for dimension $d \geq 2$ it has a ground state of both charge-density wave (CDW) order and superconductivity (SC) when half-filled. We shall show how an effective action for low energy excitations around such a ground state can be derived directly from the spontaneous breakdown of the SO(4) symmetry of the model [6,7,8], and that there must exist a new kind of skyrmion textures associated with this breakdown.

Let us consider the $d$-dimensional ($d = 2$ or 3) Hubbard model on a square or cubic lattice. The Lagrangian reads (summation convention on repeated indices assumed)

$$L = \sum_x c_{\sigma}^\dagger(x, t)i\partial_t c_\sigma(x, t) + t \sum_{\langle xx'\rangle} \left[ c_{\sigma}'(x, t)c_{\sigma}(x', t) + h.c. \right] - U \sum_x n_{\uparrow}(x, t)n_{\downarrow}(x, t),$$

where $c_\sigma(x, t)$ and $c_{\sigma}^\dagger(x, t)$ respectively annihilates and creates electrons with spin $\sigma$ ($=\uparrow, \downarrow$) at site $x = (x_1, \ldots, x_d)$ and time $t$, and $n_{\sigma}(x) = c_{\sigma}^\dagger(x)c_\sigma(x)$ (no summation). Hopping is restricted to nearest neighbors, as indicated by the bracket $\langle xx'\rangle$, with $t$ the (constant) transferring matrix element. The constant $U$ is the on-site Hubbard interaction. This is a standard theory for electrons in well-localized atomic orbitals with a probability $t$ for transitions between neighboring atoms. By now it is well known that the Hubbard model at half-filling has SO(4)$\simeq$ SU(2)$_C \times$ SU(2)$_S/Z_2$ symmetry [6,7,8], where SU(2)$_S$ corresponds to spin rotational invariance and SU(2)$_C$ (sometimes called pseudospin group [9]) contains the ordinary U(1)$_C$ charge symmetry as a subgroup. To see the SO(4) symmetry of the Lagrangian (1) in a manifest way, we use the matrix representation as introduced by Affleck [6] and Schulz [8],

$$\Psi(x, t) = \begin{pmatrix} c_{\uparrow}(x, t) \\ c_{\downarrow}(x, t) \\ (-)^x c_{\uparrow}^\dagger(x, t) \\ (-)^x c_{\downarrow}^\dagger(x, t) \end{pmatrix},$$

where we have adopted the notation $(-)^x \equiv (-)^{\sum_i x_i}$. (As usual, the lattice spacing is taken to be unit.) An ordinary spin SU(2)$_S$ transformation corresponds to
right multiplication of $\Psi$ by an SU(2)$_S$ matrix $U$: $\Psi \to \Psi U$, while the pseudospin SU(2)$_C$ transformation is left multiplication: $\Psi \to \tilde{U}\Psi$. Obviously, the latter generates the electron-hole transformation. At half-filling, defined by $\sum_{x\sigma} n_\sigma(x) = \sum_x 1$, the Lagrangian can be rewritten in terms of $\Psi$:

$$L = \sum_x \frac{1}{2} \text{tr}[\Psi^\dagger i\partial_t \Psi] + t \sum_{\langle xx' \rangle} \text{tr}[\Psi^\dagger(x,t)\Psi(x',t)]$$

$$- \frac{U}{24} \sum_{x\alpha} \left( \text{tr}[-(-)^x \Psi^\dagger \sigma_\alpha \Psi] \right)^2,$$

where $\sigma_\alpha (\alpha = 1, 2, 3)$ are the Pauli matrices. The theory now is manifestly SU(2)$_C \times$ SU(2)$_S$ invariant. The interaction term in Eq. (3) is devised in such a way to our later purpose of studying superconductivity and CDW order (although obviously it can be written in several equivalent forms). By Noether’s method we may derive from this Lagrangian the conserved spin and pseudospin charges,

$$\vec{S} = \sum_x \frac{1}{4} \text{tr}[\Psi^\dagger \Psi \vec{\sigma}] = \sum_x \frac{1}{2} \{ c_\uparrow^\dagger c_\downarrow + \text{h.c.} , i c_\uparrow^\dagger c_\downarrow + \text{h.c.} , c_\downarrow^\dagger c_\uparrow - c_\uparrow^\dagger c_\downarrow \},$$

$$\vec{J} = \sum_x \frac{1}{4} \text{tr}[\Psi^\dagger \vec{\sigma} \Psi] = \sum_x \frac{1}{2} \{ (-)^x (c_\downarrow^\dagger c_\uparrow + \text{h.c.}) , (-)^x (ic_\downarrow^\dagger c_\uparrow + \text{h.c.}) , c_\sigma^\dagger c_\sigma - 1 \},$$

which are the generators respectively of spin and pseudospin symmetries. ($J_3$ may be identified as the ordinary U(1)$_C$ charge generator apart from a constant.) The quantum operators $\vec{S}$ and $\vec{J}$ satisfy the commutation relations: $[S_a, S_b] = i\epsilon_{abc} S_c$, $[J_a, J_b] = i\epsilon_{abc} J_c$, and $[S_a, J_b] = 0$.

The SO(4) symmetry can be spontaneously broken in various patterns (see Table 1). Several authors [10,11,12] showed that spin textures (skyrmions) can exist in an antiferromagnetic (Néel) background on a square lattice. In fact, such skyrmions are associated with the spontaneously breakdown of the spin rotational symmetry SU(2)$_S$ to U(1)$_S$, as exhibited by the O(3) $\sigma$-model [13]. Yet, we shall explore an alternative case of SU(2)$_C$ broken to a ‘hidden’ U(1) subgroup (not U(1)$_C$ in general), for which the superconducting and CDW long-range orders coexist [5].

We now proceed to derive an effective field theory of low energy excitations. In the path-integral formalism, the action functional is given by the same form as Eq. (3) except replacing the electron annihilation and creation operators by the Grassmann fields (acting like anticommuting $c$-numbers): $c_\sigma \to \psi_\sigma$ and $c_\sigma^\dagger \to \psi_\sigma^\dagger$. By Hubbard-Stratonovich transformation we can cancel the four-fermion interaction term in Eq. (3) by adding to the Lagrangian a term $\Delta L = - \frac{2U}{3} \sum_{x\alpha} \langle \phi_\alpha - \frac{1}{4} \text{tr}[(-)^x \Psi^\dagger \sigma_\alpha \Psi] \rangle^2$ (for
negative $U$), where we have introduced three auxiliary scalar fields $\phi_a$. Then,

$$
L = \sum_x \left\{ \psi^{\dagger}_\sigma i \partial_t \psi_\sigma + \frac{2U}{3} \phi_a \phi_a - \frac{U}{3} \phi_a \text{tr}((-)^x \Psi^{\dagger} \sigma_a \Psi) \right\} 
+ t \sum_{(xx')} \left[ \psi^{\dagger}_\sigma (x, t) \psi_\sigma (x', t) + \text{h.c.} \right].
$$

(6)

Integrating out the $\phi_a$ fields shall return $L$ to the original form. The Lagrangian (6) is stationary in ‘field’ space at the point

$$
\vec{\phi}_0(x, t) = \frac{1}{4} \text{tr}((-)^x \Psi^{\dagger} \vec{\sigma} \Psi) 
= \frac{1}{2} \left\{ \psi_\uparrow \psi_\uparrow + \text{h.c.}, i \psi_\downarrow \psi_\uparrow + \text{h.c.}, (-)^x \psi^{\dagger}_\sigma \psi_\sigma \right\}.
$$

(7)

The expression of $\vec{\phi}_0$ infers that $\vec{\phi}$ is a three-vector in pseudospin space but transforms as a scalar under the spin group SU(2)$_S$ [14].

Now that the Lagrangian (6) is quadratic in fermion fields $\psi_\sigma$ and $\psi^{\dagger}_\sigma$, one can formally integrate out all of them and obtain the effective action for the fields of $\phi_a$, which represent the collective modes associated with ‘pseudospin’ fluctuations. Along this direction, one can follow a standard procedure (see, e.g., Sec. 3.4 of Ref. [13]). However, we shall derive the low energy effective field theory with an alternative approach, in which the role of symmetry breaking will be evident, based on such an argument: the Lagrangian (6) is SU(2)$_C$ invariant, and hence any effective action derived from it must be also SU(2)$_C$ invariant (no matter whether realized linearly or nonlinearly). Thus, together with time-reversal symmetry and parity, the SU(2)$_C$ invariance requires that the (continuum-limit) effective action for $\vec{\phi}$ be given in the following general form

$$
I_{\text{eff}} = \int d^d x dt \left[ -c_1 \vec{\phi} \cdot i \partial_t \vec{\phi} + \frac{1}{2} c_2 \partial_i \vec{\phi} \cdot \partial_i \vec{\phi} - \frac{1}{2} c_3 \partial_i \vec{\phi} \cdot \partial_j \vec{\phi} + \cdots - \mathcal{V}(\vec{\phi}) \right],
$$

(8)

$$
\mathcal{V}(\vec{\phi}) = d_2 \vec{\phi} \cdot \vec{\phi} + d_4 (\vec{\phi} \cdot \vec{\phi})^2 + \cdots,
$$

(9)

where space index $i$ runs from 1 to $d$. The terms indicated by ‘$\cdots$’ will contain higher powers of the $\vec{\phi}$ fields and/or their derivatives. All coefficients ($c_1$, $\cdots$, and $d_2$, $\cdots$) are assumed real and finite after renormalization [15].

With the ground state pointing in some specific direction in pseudospin space $\langle \vec{\phi} \rangle = \vec{\Delta} \neq 0$, the pseudospin SU(2)$_C$ symmetry is spontaneously broken down, whereas the ordinary spin SU(2)$_S$ rotational invariance is preserved but rather realized
trivially. (Recall that \( \vec{\phi} \) and \( \vec{\Delta} \) transform as scalars under SU(2)\(_S\).) By Eq. (7),

\[
\Delta_1 \equiv \frac{1}{2} \langle \psi_\downarrow \psi_\uparrow + \psi_\uparrow^\dagger \psi_\downarrow^\dagger \rangle, \quad \Delta_2 \equiv \frac{i}{2} \langle \psi_\downarrow \psi_\uparrow - \psi_\uparrow^\dagger \psi_\downarrow^\dagger \rangle \quad \text{and} \quad \Delta_3 \equiv \frac{1}{2} \langle (-)^x \psi_\uparrow^\dagger \psi_\downarrow \rangle,
\]

and they are naturally interpreted as the pairing fields and CDW order parameter. This is a manifestation of the fact that CDW order and superconductivity can coexist in the negative-\( U \) Hubbard model at half-filling for \( d \geq 2 \) \cite{5}. Nevertheless, the ground state of \( \langle \vec{\phi} \rangle = \vec{\Delta} \) is still invariant under SO(2) \( \simeq \text{U}(1) \) rotations about the direction of \( \vec{\Delta} \). This unbroken ‘hidden’ \( \text{U}(1) \) subgroup is however generally not the same as the ordinary \( \text{U}(1)_C \) charge symmetry. Clearly, a transformation of SU(2)\(_C\) can rotate the SC pairing fields \( \Delta_{1,2} \) and the CDW order parameter \( \Delta_3 \) into one another \cite{16}.

Thus, the coexistence of SC and CDW can be perfectly understood as a result of the breakdown of SU(2)\(_C\) \( \rightarrow \text{U}(1) \times \text{SU}(2)_S \) with the order-parameter space topologically regarded as a 2-sphere manifold \( S_2 \).

Since the action (8) is SU(2)\(_C\) invariant, it is always possible to rotate the pseudospin ‘field’ space in such a way that \( \vec{\Delta} \) aligns into the three-direction (\( z \)-direction) in the new ‘field’ space. We then express the \( \vec{\phi} \) field as a pseudospin rotation \( R \) acting on a three-vector \((0, 0, \sigma)\) whose first two components vanish: \( \phi_a(x, t) = R_{a3}(x, t)\sigma(x, t) \) with \( R_{ab} \) \((a, b = 1, 2, 3)\) an orthogonal matrix \( R^T(x, t)R(x, t) = 1 \). In place of the field variables \( \phi_a \), our variables now are \( \sigma(x, t) \) and whatever other variables are needed to parameterize the rotation \( R \). Let us simply choose those parameters as the \( R_{a3}(x, t) \) themselves but rather call them \( \Omega_a(x, t) \) hereafter. By definition, \( \Omega_a \) represent the Goldstone mode degrees of freedom for the pseudospin fluctuations. Furthermore, as far as the lowest energy excitations are concerned, we may simply replace \( \sigma(x, t) \) with its mean-field value \( |\vec{\Delta}| \equiv \sqrt{\Delta_a \Delta_a} \). The effective action (8) then becomes

\[
I_{\text{eff}} = \int d^d x d t \frac{c_2}{2} |\vec{\Delta}|^2 \left[ (\partial_i \vec{\Omega})^2 - \frac{c'}{c_2} \partial_i \vec{\Omega} \cdot \partial_i \vec{\Omega} + \cdots \right]
\]

with a constraint \( \vec{\Omega} \cdot \vec{\Omega} = 1 \). This is the familiar nonlinear O(3) \( \sigma \)-model. It exhibits that two gapless Goldstone modes appear around the CDW and superconductivity background along with the spontaneous breakdown of SU(2)\(_C\) \( \times \text{SU}(2)_S \) \( \rightarrow \text{U}(1) \times \text{SU}(2)_S \), as required by the Goldstone theorem \cite{17}. We remark that the result is true for \( d \geq 2 \) space dimensions only \cite{18}.

The effective field theory described by Eq. (11) can predict the existence of a topological object, known as skyrmion. To see this, consider the energy of a static
solution
\[ E = \frac{c'_2 |\vec{\Delta}|^2}{2} \int d^d x \partial_i \Omega_a \cdot \partial_i \Omega_a + \cdots \] (12)

Field configurations of finite \( E \) must have \( \partial_i \Omega_a(x) \) vanishing at spatial infinity faster than \( |x|^{-d/2} \) (where \( |x| \equiv \sqrt{x_i x_i} \)), so that \( \Omega_a(x) \) must approach a constant \( \Omega_{a\infty} \) as \( x \to \infty \) with a remainder vanishing faster than \( |x|^{(2-d)/2} \). The fields \( \Omega_a \) at any point form a homogeneous space, the (order-parameter) coset space of \( SU(2)_C \times SU(2)_S / U(1) \times SU(2)_S \simeq SO(3)/SO(2) = S_2 \) (2-sphere), for which it is possible to transform any one field value to any other by a transformation of \( SU(2)_C \). The field \( \Omega_a(x) \) thus represents a mapping of the whole \( d \)-dimensional space, with the sphere \( r = \infty \) taken as a single point, into the manifold \( S_2 \) of all field values. Therefore, finite-energy static configurations \( \Omega_a(x) \) in \( d \) space dimensions may be classified according to the \( d \)th homotopy group of \( S_2 \), \( \pi_d(S_2) \) (for a lucid discussion, see, e.g., Chap. 23 of Ref. [17]).

First, let us consider \( d = 2 \) case. The second homotopy group \( \pi_2(S_2) = \mathbb{Z} \) where \( \mathbb{Z} \) is the group of integers. Therefore, there exist skyrmions characterized by an integral winding number \( Q \) (equally called topological charge as well), which can be expressed as
\[ Q = \frac{1}{8\pi} \int d^2 x \epsilon_{ij} \vec{\Omega} \cdot (\partial_i \vec{\Omega} \times \partial_j \vec{\Omega}) \]

A skyrmion with winding number \( Q \) has energy \( E = 4\pi c'_2 |\vec{\Delta}|^2 |Q| \), and its analytical solution is already known [19]. For example, the solution for a skyrmion of winding number \( Q = 1 \) and scale \( \lambda \) reads
\[ \Omega_{1,2}(x) = \frac{4\lambda x_{1,2}}{x^2 + 4\lambda^2}, \quad \text{and} \quad \Omega_3(x) = \frac{x^2 - 4\lambda^2}{x^2 + 4\lambda^2} \]

As of \( d = 3, \pi_3(S_2) = \mathbb{Z} \). Hence, the theory also predicts the existence of pseudospin textures (skyrmions) classified by an integral winding number. Strictly speaking, the functional (12) however does not have skyrmion stationary points for \( d = 3 \), unless we add terms involving higher powers of \( \partial_i \Omega_a \) to the integrand, as indicated by ‘\( \cdots \)’. For instance, a four-derivative term will be sufficient [20].

One can gain an insight into the pseudospin skyrmions by comparing the pseudospin \( \vec{J} \) with the ordinary spin \( \vec{S} \) as defined in Eqs. (5) and (4), respectively. The Hubbard Lagrangian (1) is invariant under the combined action of the Lieb–Mattis canonical transformation defined by \( c_\uparrow(x) \rightarrow c_\uparrow(x), \ c_\downarrow(x) \rightarrow (-)^x c_\downarrow(x) \), and the reversal of interaction sign \( U \rightarrow -U \) [21]. Meanwhile, the Lieb–Mattis transformation
maps $\vec{J}$ onto $\vec{S}$. For $U > 0$, the ground state is antiferromagnetic with $\langle \vec{S} \rangle \neq 0$, which spontaneously breaks the ordinary spin symmetries, and the (spin) skyrmions are known to exist. By contrast, when $U < 0$, the ground state is in the phase of SC and CDW with $\langle \vec{J} \rangle \neq 0$, which spontaneously breaks the pseudospin symmetries, and consequently there appear pseudospin skyrmions. (Table 1 summaries the analogy between the two cases.)

The skyrmion configuration shall become unstable if the SO(4) symmetry is approximate. This happens when the Hubbard model is doped slightly away from half-filling. Then, a chemical potential term needs to be included in the Lagrangian (Eqs. 1 and 3):

$$L_{\text{break}} = -\mu \sum_x c_\sigma^\dagger c_\sigma = -2\mu J_3 + \text{Const.},$$

which when $\mu \neq 0$ explicitly breaks the SO(4) symmetry down to the obvious $U(1)_C \times SU(2)_S$ subgroup. Since the Lieb–Mattis transformation maps $J_3$ into $S_3$, this explicit breakdown of symmetry can be better viewed as caused by a ‘fictitious magnetic field’, namely, $\mu$. The presence of $L_{\text{break}}$ will somehow modify the effective action (11) and a detailed discussion shall be given elsewhere. Nevertheless, according to our understanding of spontaneously broken approximate symmetries, there are two immediate consequences of it. One is that the Goldstone modes become massive. (The usual phase mode associated with $U(1)_C$ however remains massless.) Another is that skyrmion configurations are allowed to unwrap. Imagine to do the following experiment. One first creates skyrmions with some winding number in the ground state and then starts doping the system. We conjecture that the ‘fictitious magnetic field’ $\mu$ should cause the skyrmions to unwrap but there will be some energy barrier to make it slow [22]. By contrast, the spin skyrmion texture in an antiferromagnetic background differs from the pseudospin skyrmion here in that the former is topologically stable against doping.

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[13] See, e.g., E. Fradkin, Field Theories of Condensed Matter Systems (Addison-Wesley, Redwood City, Calif., 1991).

[14] By writing back $\phi_{0a}$ in terms of $c^a_\sigma$ and $c^{\dagger}_\sigma$, one can easily verify that the resultant $\phi_{0a}$ operators form an irreducible tensor of rank 1 under the SU(2)$_C$ algebra defined by the quantum operators $\vec{J}$ — a result proved by Zhang [9].

[15] This is a standard argument in the effective field theory approach to spontaneous symmetry breaking. See, for instance, Weinberg [17].

[16] J. P. Wallington and J. F. Annett, Phil. Mag. B 76, 815 (1997).
[17] See, e.g., S. Weinberg, *The Quantum Theory of Fields II: Modern Applications* (Cambridge University Press, Cambridge, England, 1996), Chap. 19.

[18] Recall that the Mermin–Wagner–Coleman theorem forbids the spontaneous breakdown of any continuous global symmetry in $1+1$ space-time dimensions at zero temperature.

[19] For a review, see R. Rajaraman, *Solitons and Instantons* (North-Holland, Amsterdam, 1982).

[20] In the absence of such terms, any topologically non-trivial field configurations will have a continuum of values for $E$, extending down to a lower bound $E = 0$ at which $\vec{\Omega}$ becomes singular, so topology cannot stabilize such configurations. This is generally known as Derrick’s theorem. See G. H. Derrick, J. Math. Phys. 5, 1252 (1964).

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Table 1: Comparison of two possible patterns of symmetry breaking. Here, the Néel vector $\vec{M} \equiv \langle (-)^x \vec{S}(x) \rangle$ and $\vec{\Delta}$ is defined in Eq. (10).

| Properties                  | $U > 0$                  | $U < 0$                  |
|-----------------------------|--------------------------|--------------------------|
| Unbroken subgroup           | SU(2)$_C \times$U(1)$_S$ | U(1)$\times$SU(2)$_S$   |
| Broken symmetries           | Two of $S_a$’s           | Two of $J_a$’s           |
| Phase                       | Néel                     | SC+CDW                   |
| Order parameter             | $|\vec{M}|$               | $|\vec{\Delta}|$         |
| Skyrmion ($d = 2$)          | Spin texture             | Pseudospin texture       |
| Stability vs doping         | Stable                   | Unwrap                   |