

Spin Waves and Topological Terms in the Mean-Field Theory of Two-Dimensional Ferromagnets and Antiferromagnets

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(Received 4 April 1988)

We look for possible topological terms in a mean-field Lagrangian for ferromagnets and antiferromagnets inspired by the Hubbard model and study their physical effects. A topological term corresponding to Berry's phase causes the order parameter to behave like a spin moment. We find that the Hopf term is not induced and thus there is no evidence for a neutral fermion in this theory.

PACS numbers: 75.10.Lp, 02.40.+m, 11.10.Lm

The nearly half-filled Hubbard model defined on a two-dimensional square lattice

$$H = t \sum_{\langle ij \rangle} (c_i^\dagger c_j + \text{H.c.}) + U \sum c_i^\dagger c_i^\dagger c_i^\dagger c_i \quad (1)$$

has attracted a lot of attention as a possible model for high- T_c superconductors.¹ Here, c_i is a spin-doublet operator,

$$c_i = \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix},$$

annihilating an electron at site i . The symbol $\langle ij \rangle$ indicates that i and j are nearest neighbors. At half filling (i.e., with one electron per site), the mean-field theory of the Hubbard model is obtained by approximating the on-site interaction by

$$\begin{aligned} U \sum c_i^\dagger c_i^\dagger c_i^\dagger c_i &\approx U \sum c_i^\dagger c_i \langle c_i^\dagger c_i \rangle + U \sum c_i^\dagger c_i \langle c_i^\dagger c_i \rangle \\ &\quad - U \sum \langle c_i^\dagger c_i \rangle \langle c_i^\dagger c_i \rangle \\ &= U \sum_i \xi_i c_i^\dagger \sigma^3 c_i + U \sum \xi_i^2, \end{aligned}$$

where $\langle c_i^\dagger c_i \rangle = \frac{1}{2} + \xi_i$ and $\langle c_i^\dagger c_i \rangle = \frac{1}{2} - \xi_i$. This leads us to consider the effective Lagrangian

$$L_e = \sum_i c_i^\dagger (i \partial_t) c_i - t \sum_{\langle ij \rangle} (c_i^\dagger c_j + \text{H.c.}) + \Delta \sum_i \mathbf{n}_i \cdot c_i^\dagger \sigma c_i \quad (2)$$

with $\Delta = U |\xi_i|$ and $\mathbf{n}_i^2 = 1$. We have taken ξ_i to be effectively a constant but allowed the order parameter $\langle c_i^\dagger \sigma c_i \rangle$ to point in directions other than $\hat{\mathbf{e}}_z$. In (2) we regard the electrons as fast variables and the mean-field \mathbf{n}_i as slow variables; we will integrate out the electrons to obtain the effective dynamics of the mean-field order parameter. This procedure is based on the assumption that the mean-field approximation is valid. After integrating out the electrons, we will find that the energy scale for the dynamics of \mathbf{n}_i is of order t^2/Δ in the large- Δ (i.e., large U) limit, a scale much smaller than the energy scale Δ of the electronic excitations. Thus, mean-field theory is at least self-consistent. Naively, one may want

to describe the dynamics of \mathbf{n}_i phenomenologically by

$$L_n = \frac{1}{2g^2} \sum \dot{\mathbf{n}}_i \cdot \dot{\mathbf{n}}_i - J \sum_{\langle ij \rangle} \mathbf{n}_i \cdot \mathbf{n}_j. \quad (3)$$

At first sight, L_n does not appear to describe the dynamics of spin variables since spin variables should satisfy an equation of motion that is first order in time. However, as we will see, because of its coupling to the electrons, \mathbf{n}_i does take on the characteristics of a spin variable at low frequencies.

For simplicity, we first consider the properties of the model described by Eq. (2) and Eq. (3) in the limit $\Delta \gg t$ and at half filling. In this limit, the electron spectrum has a large energy gap of order Δ at the Fermi surface. In particular, for $t=0$, the ground state consists of one electron per site with its spin parallel (antiparallel) to \mathbf{n} if $\Delta > 0$ (< 0). One may thus naively expect that the electrons have little effect on low-energy physics and may be integrated out leaving the Lagrangian L_n .

However, as has been demonstrated in continuum field-theoretic models, namely, nonlinear σ models coupled to Dirac fermions, various topological terms may be induced and they survive even when the fermion mass—the analog of U here—goes to infinity. These topological terms can alter the low-energy properties of the model dramatically. In particular, in the (2+1)-dimensional O(3) nonlinear σ model described by the action $\mathcal{L}_\sigma = (\partial_\mu n^a)^2 / 2f^2$, where $a=1,2,3$ are O(3) isospin indices, a Hopf term² may be added. In general, the addition of a Hopf term to a (2+1)-dimensional theory can endow the relevant excitations in the theory with fractional angular momentum and statistics.^{2,3} Let us remind the reader that in field theory the Hopf term is constructed by adding the terms

$$\int d^3x g \epsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda + \int d^3x A_\mu J^\mu$$

to the action, where J^μ is the topological current

$$J^\mu = \epsilon^{\mu\nu\lambda} \epsilon_{abc} n^a \partial_\nu n^b \partial_\lambda n^c.$$

Eliminating A_μ , we obtain the nonlocal Hopf term

$$\mathcal{H} \sim \int d^3x d^3y \epsilon^{\mu\nu\lambda} J_\mu(x) [(x-y)_\nu / |x-y|^3] J_\lambda(y).$$

It turns out that the Hopf term becomes local

$$\mathcal{H} \sim \int d^3x \epsilon^{\mu\nu\lambda} (z^\dagger \partial_\mu z) (\partial_\nu z^\dagger \partial_\lambda z)$$

when rewritten in terms of $z = (z_1, z_2)$, the spinor "square root" of $n(x)$ defined by $n(x) = z^\dagger(x) \sigma z(x)$, $z^\dagger z = 1$. The Hopf term can also be induced⁴ by coupling $n^a(x)$ to an isodoublet Dirac fermion as in the Lagrangian $\mathcal{L}_\psi = \bar{\psi}(i \not{\partial} - mn^a \tau^a) \psi$. The coefficient of the induced Hopf term is such that a soliton in the model is changed from a boson to a fermion.

A number of people have speculated recently that such electrically neutral fermions may appear in the Hubbard model.⁵ It is thus of some interest to study the appearance of topological terms in the Lagrangian L .

Before we begin, we remark that any possible connection between the lattice model and the field-theory model studied in Refs. 2-4 is far from obvious even though L_n and L_e resemble \mathcal{L}_σ and \mathcal{L}_ψ . It is well known that Dirac fermions cannot be put on the lattice without doubling.

The dynamics of the electrons is described by the Hamiltonian

$$H_e = t \sum_{\langle ij \rangle} c_i^\dagger c_j + \text{H.c.} - \Delta \sum \mathbf{n}_i \cdot c_i^\dagger \sigma c_i. \quad (4)$$

If the background field $\mathbf{n}_i(t)$ varies slowly in time, we may use the adiabatic approximation to calculate the low-energy effective Lagrangian. In this approximation, the effects of the electrons consist of two terms. The first comes from the ground-state energy of the instantaneous Hamiltonian

$$H(t) | \Psi_0(t) \rangle = E_0(t) | \Psi_0(t) \rangle.$$

The second term is the Berry's phase,⁶ originating in the time dependence of the ground-state wave function

$$i\Gamma = \langle \Psi_0(t) | \frac{d}{dt} | \Psi_0(t) \rangle.$$

In the $t/\Delta = 0$ limit, or equivalently, to leading order in $1/\Delta$, the ground state $|\Psi_0(t)\rangle = \otimes_i |\mathbf{n}_i\rangle \equiv \otimes_i (z_{i1} c_{i\uparrow}^\dagger + z_{i2} c_{i\downarrow}^\dagger) |0\rangle$ where $z_i = (z_{i1}, z_{i2})$ is the spinor "square root" of \mathbf{n}_i defined by $\mathbf{n}_i = z_i^\dagger \sigma z_i$, $z_i^\dagger z_i = 1$. In other words, the ground state consists of one electron at each site with its spin parallel to \mathbf{n}_i , that is, $\mathbf{n}_i \cdot c_i^\dagger \sigma c_i | \mathbf{n}_i \rangle = | \mathbf{n}_i \rangle$. The ground-state energy to leading order $E_0 = -\Delta N$ (with N the number of lattice sites) is independent of $\mathbf{n}_i(t)$. The Berry's phase associated with the ground state is given by $\Gamma = -i \sum_i z_i^\dagger \dot{z}_i$. Thus, in this order, the effective Lagrangian is

$$L_{\text{eff}} = \frac{1}{2g^2} \sum \dot{\mathbf{n}}_i \cdot \dot{\mathbf{n}}_i - J \sum_{\langle ij \rangle} \mathbf{n}_i \cdot \mathbf{n}_j + i \sum_i z_i^\dagger \dot{z}_i. \quad (5)$$

Note that the strength of the Berry term is fixed.

To study the physical effects of this extra topological term, consider the spin-wave spectrum. While $z^\dagger \dot{z}$ cannot be expressed simply in terms of \mathbf{n} , its variation can

be written as

$$\int dt \delta(z^\dagger \dot{z}) = \frac{1}{2} i \int dt \delta \mathbf{n} \cdot (\mathbf{n} \times \dot{\mathbf{n}}).$$

We have the equation of motion

$$(\delta_{\alpha\beta} - n_{i\alpha} n_{i\beta}) \left(g^{-2} \ddot{n}_{i\beta} + 2J \sum_j n_{j\beta} \right) + \frac{1}{2} (\mathbf{n}_i \times \dot{\mathbf{n}}_i)_\alpha = 0, \quad (6)$$

where the summation runs over the sites j that are nearest neighbor of the site i . Expanding in small fluctuations around the antiferromagnetic state ($J > 0$), $\mathbf{n}_i = (-1)^i \hat{\mathbf{e}}_z + \delta \mathbf{n}_i$, and going to frequency and momentum space, we find

$$\begin{pmatrix} -\omega^2/g^2 + f(k) & -\frac{1}{2} i\omega \\ \frac{1}{2} i\omega & -\omega^2/g^2 + f(k+Q) \end{pmatrix} \begin{pmatrix} \delta n_k^1 \\ \delta n_{k+Q}^1 \end{pmatrix} = 0, \quad (7)$$

where $f(k) = 4J[2 + \cos(k_x a) + \cos(k_y a)]$, a is the lattice spacing, and $Q = (\pi/a, \pi/a)$ is the vector to a corner of the Brillouin zone. A similar equation connects δn_k^2 and δn_{k+Q}^2 . For small k , the dispersion relation has a high-frequency branch $\omega^2 \approx 16Jg^2(1 + g^2/64J) - O(k^2)$ and a low-frequency spin-wave branch $\omega^2 = (ka)^2 \times (2Jg^2)/(1 + g^2/64J)$. Were the Berry term absent, then the factor $(1 + g^2/64J)$ would be replaced by unity. Thus, topological effects modify the spin-wave velocity but do not alter the spin wave qualitatively.

We can regard L_{eff} in (5) as a phenomenological Lagrangian and discuss in passing a ferromagnetic system ($J < 0$). Such an effective Lagrangian may arise from a modified Hubbard model obtained by our adding a spin interaction $J' \sum_{\langle ij \rangle} c_i^\dagger \sigma c_i c_j^\dagger \sigma c_j$ to the Hamiltonian in (1). Expanding around the ferromagnetic ground state $\mathbf{n}_i = \hat{\mathbf{e}}_z + \delta \mathbf{n}_i$, we find

$$\begin{pmatrix} -\omega^2/g^2 + h(k) & -\frac{1}{2} i\omega \\ \frac{1}{2} i\omega & -\omega^2/g^2 + h(k) \end{pmatrix} \begin{pmatrix} \delta n_k^1 \\ \delta n_k^2 \end{pmatrix} = 0, \quad (8)$$

with $h(k) = 4J[2 - \cos(k_x a) - \cos(k_y a)] = f(k+Q)$. The spin wave has two branches described by $(\delta n_k^1, \delta n_k^2) \propto (1, \pm i)$ and with the dispersion relations $\omega = [\frac{1}{16} g^4 + g^2 h(k)]^{1/2} \pm \frac{1}{4} g^2$. For small k , one of these branches has a low-frequency spin wave with $\omega \approx 4J(ka)^2$. We note that here, were the Berry term absent, that is, were the off-diagonal entry absent in Eq. (8), the dispersion relation would be linear $\omega \propto k$ rather than quadratic $\omega \propto k^2$. Thus, topological effects are crucial in this model to produce the spectrum expected on general grounds.⁷

Another way of expressing this is that the Berry term restores to the variable \mathbf{n} its spin characteristic. At low frequencies, in the ferromagnetic case, we can ignore the $\ddot{\mathbf{n}}$ term in Eq. (6) and obtain the equation

$$\dot{\mathbf{n}}_i = 4J \left(\mathbf{n}_i \times \sum_j \mathbf{n}_j \right). \quad (9)$$

In the antiferromagnetic case, for (9) to hold, we have to take the $g^2 \rightarrow \infty$ limit. Equation (9) is precisely the equation appropriate for a spin moment. Alternatively, instead of L_n as in (3), we could have taken for L_n the last two terms in (5).

We can now compute perturbatively in the hopping coefficient t : To lowest order we find an antiferromagnetic $\Delta L_n = -(t^2/2\Delta) \sum_{(ij)} \mathbf{n}_i \cdot \mathbf{n}_j$ to the effective Lagrangian.

Now we want to ask whether the solitons in the antiferromagnetic state are fermions or have fractional spin statistics, i.e., whether the Hopf term appears in the effective Lagrangian of \mathbf{n}_i after the electrons are integrated out. Although the topological term $i \sum_i z_i^\dagger \dot{z}_i$ does appear in zeroth order in $1/\Delta$, it is obviously not the Hopf term. In order to see whether the Hopf term appears in higher orders in $1/\Delta$ and/or when t is not small compared to Δ , we would like to study the theory for arbitrary Δ . This can be done by our making a canonical transformation to the electron field and expanding in the long-wavelength limit. Introducing $\psi_i = U_i c_i$, where

$$U_i = \begin{pmatrix} y_{1i}^* & y_{2i}^* \\ -y_{2i} & y_{1i} \end{pmatrix}, \quad (10)$$

with $y_i = z_i$ for $(-1)^i = +1$ and $y_i = \sigma_2 z_i^*$ for $(-1)^i = -1$ so that $\mathbf{n}_i \cdot \boldsymbol{\sigma} = U_i^\dagger \sigma_3 U_i (-1)^i$, we can rewrite the Lagrangian L_e as $L_e = L_0 + L_1$, where

$$L_0 = i \sum_i \psi_i^\dagger \partial_t \psi_i - t \sum_{(ij)} \psi_i^\dagger \psi_j - \Delta \sum_i \psi_i^\dagger \sigma_3 \psi_i (-1)^i$$

and

$$L_1 = -t \sum_{(ij)} \psi_i^\dagger \xi_{ij} \psi_j + \sum_i \psi_i^\dagger v_i \psi_i,$$

with $\xi_{ij} = U_i U_j^\dagger - 1 = \xi_{ji}^\dagger$ and $v_i = i U_i \partial_t U_i^\dagger$. This is clearly a lattice gauge theory with $A_0(i)$ corresponding to $-iv_i$, $A_1(i)$ to $\xi_{i,i+\hat{x}}/a$ and $A_2(i) = \xi_{i,i+\hat{y}}/a$. In the continuum limit, $A_\alpha = U \partial_\alpha U^\dagger$, $\alpha=0,1,2$. L_0 can be diagonalized exactly. For long-wavelength fluctuations around the antiferromagnetic state, L_1 is small and can be treated as a perturbation. The effective Lagrangian of \mathbf{n}_i may be calculated in a power expansion of v_i and ξ_{ij} . Similarly, for long-wave fluctuations around the ferromagnetic state, we may choose U_i in the canonical transformation (10) to be

$$U_i = \begin{pmatrix} z_{1i}^* & z_{2i}^* \\ -z_{2i} & z_{1i} \end{pmatrix}.$$

In that case, $L_e = L'_0 + L_1$, where L'_0 is obtained from L_0

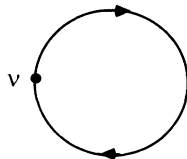


FIG. 1. Diagram which contributes to the Berry term.

by our omitting the $(-1)^i$ in the term proportional to Δ .

The topological term discovered in previous calculations is first order in v_i and may be regarded as originating from normal ordering of the second term in L_1 (Fig. 1).

In the antiferromagnetic state, the free propagator is given by

$$G_{kk'}^0 = \frac{\omega + \epsilon_k}{\omega^2 - E_k^2 + i\delta} \delta_{k-k'} + \frac{\Delta \sigma_3}{\omega^2 - E_k^2 + i\delta} \delta_{k-k'+Q},$$

where $\epsilon_k = 2t[\cos(k_x a) + \cos(k_y a)]$ and $E_k = (\epsilon_k^2 + \Delta^2)^{1/2}$. The Feynman diagram in Fig. 1 gives

$$\frac{i}{N} \left[\sum_k \frac{\Delta}{2E_k} \right] \sum_i \text{tr} v_i \sigma_3 (-1)^i = \frac{i}{N} \left[\sum_k \frac{\Delta}{E_k} \right] \sum_i y_i^\dagger \dot{y}_i (-1)^i$$

which reduces to our previous result when $\Delta \rightarrow \infty$ (or $t \rightarrow 0$) with a coefficient $\Delta/|\Delta|$.

Similarly the free propagator in the ferromagnetic state is given by

$$G^0(k) = (\omega - \epsilon_k - \Delta \sigma_3 + i\delta_k)^{-1},$$

where $\delta_k = 0^+$ if $\epsilon_k + \Delta \sigma_3 > 0$ and $\delta_k = 0^-$ if $\epsilon_k + \Delta \sigma_3 < 0$. The graph in Fig. 1 gives

$$i \frac{N_\downarrow - N_\uparrow}{N} \sum_i z_i^\dagger \dot{z}_i,$$

where N_\uparrow (N_\downarrow) is the total number of spin-up (down) electrons in the ground state. When $\Delta > 4t$, $N_\downarrow = N$ and $N_\uparrow = 0$, we obtain our old result again.

To identify the Hopf term on the lattice, we recall that in the continuum limit, the Hopf term is given by^{2,3}

$$H_1 = \int \text{tr} A^3 = \int d^3x \epsilon^{\mu\nu\lambda} \text{tr} A_\mu A_\nu A_\lambda,$$

where we have used the notation of differential form and defined the matrix one-form $A = A_\mu dx^\mu = U dU^\dagger$, $\mu=0,1,2$. Since $dA = -A^2$, this term is also proportional to the other three terms:

$$H_2 = \int d^3x \epsilon^{\mu\nu\lambda} \text{tr} A_\mu \partial_\nu A_\lambda,$$

$$H_3 = \int d^3x \epsilon^{\mu\nu\lambda} \text{tr} A_\mu \sigma^3 A_\nu \sigma^3 A_\lambda,$$

$$H_4 = \int d^3x \epsilon^{\mu\nu\lambda} \text{tr} A_\mu \sigma^3 \partial_\nu A_\lambda \sigma^3.$$

Thus, we are to identify in the effective action W the terms $W = \sum_p a_p [H_p]$ and to determine the coefficients a_p where $[H_p]$ represents the lattice version of H_p . Thus

$$[H_1] = \sum_i \text{tr} v_i [\xi_{i,i+\hat{x}}, \xi_{i,i+\hat{y}}],$$

for example.

In our model the Hopf term may arise from the three diagrams in Fig. 2. Figure 2(a) contributes to a_1 and a_3 . Figures 2(b) and 2(c) contribute to a_2 and a_4 .

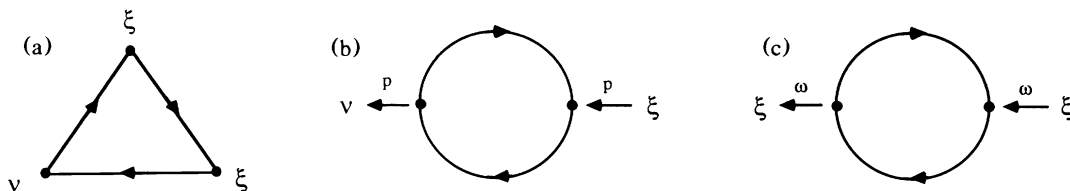


FIG. 2. Diagrams which potentially contribute to the Hopf term.

After a straightforward calculation, we find that all coefficients a_p in W are zero in both the antiferromagnetic and ferromagnetic state. For example, calculating the first term in W from Fig. 2(a), we find that

$$a_1 \propto \int \frac{d\omega}{2\pi} \sum_k \frac{(\omega + \epsilon_k)^3}{(\omega^2 - E_k^2)^3} e^{ik \cdot (\hat{x} + \hat{y})a}$$

in the antiferromagnetic state. The above expression is zero since the integrand is odd under $\omega \rightarrow -\omega$ and $k \rightarrow k + Q$. Therefore the Hopf term does not appear in the antiferromagnetic and ferromagnetic state. The soliton in the antiferromagnetic state is a neutral boson, at least for the model considered in this paper.

The calculation of the induced Hopf term in field theory amounts to our evaluating the fermion determinant in \mathcal{L}_ψ , namely, $\det(i\mathcal{D} - mn^a\tau^a)/\det(i\mathcal{D} - M)$. The regulator (with mass M) is needed to cancel the high-lying eigenvalues of $i\mathcal{D}$ (even though the relevant Feynman diagrams are apparently convergent). One way of calculating the determinant involves diagonalizing $n^a\tau^a = U\tau_3 U^{-1}$ so that we have $\det(i\mathcal{D} - m\tau^3)/\det(i\mathcal{D} - M)$, where $D_\mu = \partial_\mu + V_\mu$ and $V_\mu \equiv U^{-1}\partial_\mu U$ is a non-Abelian (pure) gauge potential. It can be verified that the numerator gives (in the notation of differential forms with $V = V_\mu dx^\mu$) terms like $\text{tr}\tau_3 V^3$, which vanishes identically, while the denominator is proportional to $(M/|M|)\text{tr}V^3$, the unique three-form on the sphere S^3 describing the Hopf invariant. In other words, the induced Hopf term comes from the regulator needed to define the theory. We have indicated that the coefficient of the Hopf term depends only on the sign of M and thus the induced effect remains even as $M \rightarrow \infty$.

One may notice that \mathcal{L}_ψ is invariant under T and P provided that $n^a \rightarrow -n^a$ under T and P . Thus one may naively expect that the P and T odd Hopf term should not appear in the low-energy effective action. But in field theory, a regulator is needed to define the theory. With the choice of the Pauli-Villars regulator $[\det(i\mathcal{D} - M)]^{-1}$, the regulated theory is not invariant under P and T . Thus, the appearance of the Hopf term is consistent with the symmetries of the (regulated) theory.

With this understanding, we see why we would not expect the appearance of a Hopf term in a lattice theory. The lattice provides a short-distance regularization which clearly violates neither P nor T . Our model Lagrangian and the ground states (ferromagnetic and anti-

ferromagnetic states) obviously also do not violate P .

In conclusion, we have found in the $t/\Delta \ll 1$ limit a topological Berry term in both the antiferromagnetic and ferromagnetic case. It will be interesting to determine what this term becomes as t/Δ increases. In the long-wavelength limit but without restriction on Δ and t , we are able to determine the absence of the Hopf term. Within the limitations of this analysis, the soliton in the theory would appear to be bosonic.

We thank R. Schrieffer for helpful discussions. This research was supported in part by the National Science Foundation under Grant No. PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration, at the University of California at Santa Barbara.

Note added.—After the submission of this paper we received copies of unpublished work from Fradkin and Stone⁸ and Haldane⁹ reaching similar conclusions. We understand that Dombre and Read, and also Fuffe and Larkin, have also reached similar conclusions. (However, we have not yet seen these papers.)

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