Topological Magnetic Solitons in the Two-Dimensional Mott-Hubbard Gap

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We derive from first principles the existence of deep level localized electronic gap states, induced by hedgehog solitons, in the two-dimensional Hubbard model. These arise naturally as excitations in a new topological magnetic condensate of the many-electron system associated with $\pi_1(SO(3))$. The condensate exhibits local spin $\frac{1}{2}$ magnetic moments as well as topological "spin flux." This flux emerges microscopically from a homotopically nontrivial phase rotation of the electron spinor field and leads to an intriguing relativistic structure for the Mott-Hubbard gap.

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The discovery of high temperature superconductivity [1] has sparked broad interest in the magnetic properties of strongly correlated electron systems. It was suggested by Anderson [2] that a spin-liquid phase of strongly interacting electrons may be responsible for many of the anomalous electronic and magnetic features observed in such systems [3]. In this paper we describe a new topological feature of the interacting electronic system in two dimensions which may give rise to such anomalies.

In a recent series of papers [4–6], we have presented a careful study of the magnetic and electronic properties of the strongly correlated Hubbard model starting from a mean field theory of spiral magnetism and continuing to the lowest order fluctuation corrections. The fluctuation Hamiltonian led to a physical picture of the doped Mott-Hubbard system as a highly nontrivial metal in which there was strong coupling between collective charge and spin excitations. The aim of this study was to isolate those normal state properties of the copper-oxide high temperature superconductors which may be associated with small fluctuations about a spiral magnetic mean field, from those which require large amplitude nonlinear corrections or an entirely new condensate at the mean field level. We found that certain features such as the twist of the magnetic background, the closure of the Mott-Hubbard gap [4,5], and the sign change of the Hall coefficient [6] with doping δ could be described in standard spin-density-wave mean field theory of the intermediate coupling Hubbard model. However, other important features such as the rapid loss of magnetic long range order with δ, the marginal Fermi-liquid behavior [7], and the striking mid-infrared absorption [8] could not be accounted for in a natural way.

In this paper we discuss the properties of a topological fluctuation correction which connects the previous mean field ground state to a possible new condensate at large doping. Unlike the standard spiral magnetic states, the many-electron wave function for this topological condensate is a Slater determinant of single electron spinor wave functions in coordinate space which change sign under 2π rotation about an axis $\hat{\mathbf{z}}$, passing through the center of any lattice plaquette. These single electron states are obtained by applying a homotopically nontrivial phase rotation to the electron spin for paths that encircle an elementary plaquette of the 2D square lattice, in addition to any rotation of the local spin orientation detectable by neutron scattering. These wave functions are physically admissible provided that the resulting phase change acquired around any plaquette is ± 1, in accordance with the topology of the rotation group SO(3). If the phase change is -1, this is formally equivalent to passing a "spin flux" of π through the plaquette. A key difference between our topological condensate and previously discussed flux phases [9] is that the phase change is in fact opposite for opposite spins. Accordingly, the currents for up and down spin electrons circulate in opposite directions, leading to zero net charge current.

An important simplification of the many-electron problem occurs if an $e^{\pm i\pi}$ phase factor is created in this manner around *each* plaquette of the 2D square lattice. The effective one-electron Hamiltonian, in this case, contains not only the usual magnetic scattering potential of the spin-density-wave mean field, but also a spin-dependent hopping matrix element. Hopping from one lattice site to a nearest neighbor is now described by an SU(2) matrix which accounts for the phase change of the electron spinor from site to site. The resulting matrices which describe hopping between unit cells in the x and y directions, respectively, satisfy an anticommutation algebra. This leads to a remarkable relativistic Dirac spectrum for low energy excitations. We derive the electronic structure of this condensate in the presence of topologically charged magnetic hedgehog solitons. These solitons describe local tunneling events between the two degenerate antiferromagnetic vacua. In addition, for unit values of topological charge, they correspond to the addition or removal of an elementary quantum of spin flux. These solitons induce localized electronic states within the relativistic Mott-Hubbard gap. Magnetic textures of this nature can be excited optically and may account for the anomalous broadband infrared absorption in high T_c superconductors. These solitons are free to move within the two-dimensional plane, greatly enhancing the destruction of long range magnetic order with doping and possibly

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leading to the marginal Fermi-liquid behavior of the normal state.

The topological structure of the many-electron Hilbert space may be described formally by considering the set of all physically admissible local gauge transformations on the Hubbard model [10,11]:

$$\mathcal{H} = -t \sum_{\substack{\langle ij \rangle \\ \alpha}} [b^\dagger_{i\alpha} b_{j\alpha} + \text{H.c.}] + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{1}$$

Here $b^\dagger_{i\alpha}$ creates an electron at site i of spin α. We consider a local gauge transformation on this operator which implements a Euler angle rotation of the electron's internal coordinate system. Denoting the three Euler angles by $\boldsymbol{\eta}_i = (\eta_{1i}, \eta_{2i}, \eta_{3i})$, we define the rotated electron operator $c^\dagger_{i\alpha}$ by the relation $b^\dagger_{i\alpha} \equiv [e^{i(\boldsymbol{\eta}_i \cdot \boldsymbol{\sigma})/2}]_{\alpha\beta} c^\dagger_{i\beta}$. Here $\boldsymbol{\sigma} \equiv (\sigma^1, \sigma^2, \sigma^3)$ are the three Pauli spin matrices and there is an implicit summation over the repeated index β. It is clear that such a substitution leaves the interaction term invariant. However, if the Euler angle field $\boldsymbol{\eta}_i$ varies with index i, the electron hopping terms will be modified. Defining a SU(2) gauge field $\mathbf{A}^\mu$ by the relation

$$(\eta_{\mu i} - \eta_{\mu j}) \sigma^\mu_{\alpha\beta} = \int_i^j d\boldsymbol{l} \cdot \mathbf{A}^\mu \sigma^\mu_{\alpha\beta}, \tag{2}$$

the gauge transformed Hamiltonian becomes

$$\mathcal{H} = \sum_{\langle ij \rangle} [c^\dagger_{i\alpha} T^{ij}_{\alpha\beta} c_{j\beta} + \text{H.c.}] + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{3a}$$

where the hopping coefficient t for the link $\langle i, j \rangle$ has been replaced by the SU(2) matrix

$$T^{ij} = -t \exp\left(i/2 \int_i^j d\boldsymbol{l} \cdot \mathbf{A}^\mu \sigma^\mu \right). \tag{3b}$$

Here, we assume for simplicity that each of the Euler angle rotations is about some fixed axis $\hat{\mathbf{n}}$.

There is a crucial difference between the nature of physically admissible gauge transformations for spin 1/2 electrons and those familiar from elementary scalar quantum mechanics. In the latter case, the wave function $\psi(\mathbf{r})$ is required to be single-valued in three-dimensional Euclidean space. A relabeling of the phase of the wave function $\psi \rightarrow \exp[i\theta(\mathbf{r})]\psi$ leads to the introduction of a U(1) gauge field into the Schrödinger equation. Provided that the gauge field is chosen to have the form $\mathbf{A} = \boldsymbol{\nabla}\theta$ for some single-valued field $\theta(\mathbf{r})$, the spectrum is unchanged. The introduction of more general configurations of the gauge field for which $\boldsymbol{\nabla} \times \mathbf{A} \neq 0$, however, corresponds to the addition of electromagnetic forces [12]. For the case of spin 1/2 electrons, the internal wave function defined on the space of Euler angles is *two-valued* [13]. There are two distinct spinors which describe the same physical state of the electron and two distinct SU(2) matrices, $\pm T$, which describe the same physical rotation of the electron's internal coordinate system. This is a direct consequence of the doubly connected topological nature of the group manifold of SO(3). It follows that the one-electron spinor wave function $\chi^+(\mathbf{r}) \equiv [\phi^*_\uparrow(\mathbf{r}), \phi^*_\downarrow(\mathbf{r})]$ describing the up and down spin amplitudes can be relabeled at each point in space by a local SU(2) gauge transformation $\chi \rightarrow T(\mathbf{r})\chi$ which creates a phase change of either ± 1 for any closed loop in the coordinate space $\mathbf{r}$. In the case of a phase change $e^{i\pi}$, it is apparent that $\boldsymbol{\nabla} \times \mathbf{A} \neq 0$. Nevertheless, such a gauge field is admissible without the introduction of an external Yang-Mills force. It does, however, describe a distinct topological sector of the many-electron Hilbert space which may be accessible in the presence of strong electron-electron interactions.

We consider a general Hartree-Fock, mean-field, factorization [4–6] of the Hubbard model in which the ground state expectation value of the electron spin operator is given by $\frac{1}{2}\langle c^\dagger_{i\alpha} \boldsymbol{\sigma}^{\alpha\beta} c_{i\beta} \rangle = s\hat{\mathbf{n}}_i$, where $\hat{\mathbf{n}}_i = \pm\hat{\mathbf{n}}(\mathbf{r})$ is a unit vector describing the orientation of the local magnetic moment at each lattice site i, and $\hat{\mathbf{n}}(\mathbf{r})$ is a slowly varying plaquette variable which defines the axis of quantization of the local antiferromagnetic ordering. For the uniform antiferromagnet one can choose $\hat{\mathbf{n}}(\mathbf{r}) = +\hat{\mathbf{z}}$. [Later, we will introduce magnetic textures by allowing $\hat{\mathbf{n}}(\mathbf{r})$ to vary slowly with $\mathbf{r}$.]

A simple topological variant of this spin-density wave state may now be obtained by associating the SU(2) matrix $T \equiv -t \exp\{i\frac{\pi}{4}[\hat{\mathbf{n}}(\mathbf{r}) \cdot \boldsymbol{\sigma}]\}$ with each directed link of the lattice as depicted in Fig. 1. With this choice it is apparent that the product of SU(2) matrices around any elementary plaquette of the 2D square lattice is equal to -1.

In the topological sector defined in Fig. 1, the unit cell now contains four lattice sites labeled $j = 1, \ldots, 4$, and accordingly we define a set of four two-component spinor fields $\chi^{+(j)}(\mathbf{r}_j) \equiv (c^\dagger_{j\uparrow}, c^\dagger_{j\downarrow})$ to describe the one-electron wave function. The mean-field Hamiltonian can now be expressed in terms of an 8-component field $\Psi^\dagger(\mathbf{r}) \equiv [\chi^{+(1)}, \chi^{+(2)}, \chi^{+(3)}, \chi^{+(4)}]$ defined on the plaquette containing $\mathbf{r}$. In addition to the usual Pauli matrices $\boldsymbol{\sigma}$, which act on the internal spin space of the electron, it is convenient to introduce two new sets of 4×4 matrices which act on the four site indices of the elementary unit cell:

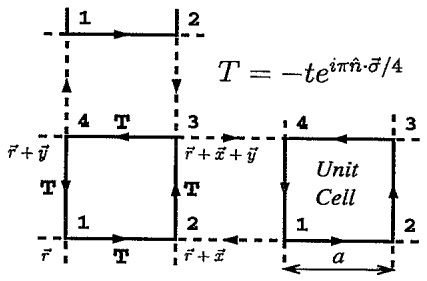

FIG. 1. Unit cell with four point basis. The spin-flux phase is obtained by associating the SU(2) matrix T (see text) with each directed link of the 2D lattice. Here $\mathbf{x} = a\hat{\mathbf{x}}$ and $\mathbf{y} = a\hat{\mathbf{y}}$.

$$\tau = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix} \tag{4a}$$

and

$$\gamma_z \equiv \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \gamma_x \equiv \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \gamma_y = i \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}. \tag{4b}$$

Clearly, the set τ and the set γ individually satisfy a cyclic Pauli spin algebra, but commute with each other: $[\tau_j, \gamma_k] = 0$ for all j and k. Using the direct tensor product of these matrices with the physical Pauli spin matrices σ (which act on the electron's *internal* wave function), it is possible to rewrite the kinetic energy term of the Hubbard Hamiltonian in the 8×8 matrix form:

$$H_0 \equiv -2t \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} [\cos(k_x a)\tilde{\alpha}_x + \cos(k_y a)\tilde{\alpha}_y]\Psi_{\mathbf{k}}, \tag{5}$$

where

$$\begin{aligned} \tilde{\alpha}_x &\equiv [\tau_x + (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})\tau_y]/\sqrt{2}, \\ \tilde{\alpha}_y &\equiv [\tau_x - (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})\tau_y]\gamma_x/\sqrt{2}, \end{aligned} \tag{6}$$

and $\Psi_{\mathbf{k}} \equiv (N)^{-1/2} \sum_{\mathbf{r}_i} e^{-i\mathbf{k}\cdot\mathbf{r}_i} \Psi(\mathbf{r}_i)$. Here a is the lattice constant, N is the number of unit cells, and the reduced Brillouin zone for the $\mathbf{k}$ summation is $|k_x|, |k_y| < \pi/2a$. Similarly, the antiferromagnetic mean-field interaction term $U \sum_i c_i^{\dagger\alpha} \langle \mathbf{s}_i \rangle \cdot \boldsymbol{\sigma}_{\alpha\beta} c_i^{\beta}$ becomes

$$H_{\text{int}}^{\text{MF}} \equiv -m \sum_k \Psi_k^{\dagger} (\tilde{\alpha}_z \gamma_x) \Psi_k, \tag{7}$$

where $\tilde{\alpha}_z \equiv -(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})\tau_z\gamma_x$ and $m \equiv U|\langle \mathbf{s}_i \rangle|$ defines the magnitude of the antiferromagnetic, Mott-Hubbard gap.

A straightforward calculation reveals that the 8×8 matrices $\boldsymbol{\alpha} \equiv (\tilde{\alpha}_x, \tilde{\alpha}_y, \tilde{\alpha}_z)$ themselves satisfy a cyclic Pauli spin algebra with $\{\tilde{\alpha}_i, \tilde{\alpha}_j\} = 2\delta_{ij}$. This implies [14] that the single electron spectrum at mean-field level has the relativistic, Dirac form $E = \pm\sqrt{4t^2[\cos^2(k_x a) + \cos^2(k_y a)] + m^2}$. The band edges for the lower and upper Mott-Hubbard bands occur at the four equivalent zone-corner points $\mathbf{k}_0 = (\pi/2a)(\pm 1, \pm 1)$. An effective, one-electron, continuum Hamiltonian may be obtained by linearizing the dispersion relation about these points and making the replacement $\mathbf{k} - \mathbf{k}_0 \rightarrow -i\boldsymbol{\nabla} \equiv -i(\partial_x, \partial_y)$:

$$\mathcal{H}_{\text{eff}} = 2ita(\tilde{\alpha}_x \partial_x + \tilde{\alpha}_y \partial_y) - m\tilde{\alpha}_z\gamma_x. \tag{8}$$

Twist of the magnetic background away from antiferromagnetic alignment from one plaquette to another may be accomplished by allowing the matrices $\boldsymbol{\alpha}$ to have slow spatial variations through the factor $\hat{\mathbf{n}}(\mathbf{r}) \cdot \boldsymbol{\sigma}$ which they contain. It is easy to verify [15] that the generalization of $\mathcal{H}_{\text{eff}}$ for any magnetic texture which varies slowly on the scale of the lattice constant is obtained by symmetrizing the kinetic energy with respect to the momentum operator $\mathbf{p} \equiv -i\boldsymbol{\nabla}$. In particular the hermiticity of $\mathcal{H}_{\text{eff}}$ is preserved for spatially varying $\hat{\mathbf{n}}(\mathbf{r})$ if we make the replacement $\boldsymbol{\alpha} \cdot \mathbf{p} \rightarrow \frac{1}{2}[\boldsymbol{\alpha} \cdot \mathbf{p} + \mathbf{p} \cdot \boldsymbol{\alpha}]$. These spatial variations, while preserving the symmetry of the eigenvalue spectrum of $\mathcal{H}_{\text{eff}}$ about $E = 0$, give rise to localized electronic states within the relativistic Mott-Hubbard gap.

We consider a general hedgehog soliton, of topological charge μ, defined by

$$\hat{\mathbf{n}}(\mathbf{r}) \cdot \boldsymbol{\sigma} = U^{\dagger}\sigma_z U, \tag{9}$$

where $U \equiv \exp[-i\sigma_y\theta(r)/2] \exp(i\mu\sigma_z\phi/2)$. Here, we have introduced polar coordinates $\mathbf{r} = (r, \phi)$ and $\theta(r)$ is a general function describing the magnetic twist in the radial direction. A straightforward but lengthy calculation reveals that the z component of the electron's total angular momentum is a constant of motion in this texture, if and only if the condition

$$\nabla\theta(r) = s_1 \mu \sin\theta(r)/r, \tag{10}$$

where $s_1 = \pm 1$ is satisfied. Remarkably, this is precisely the condition for a local minimum (instanton) of the classical magnetic energy [16], $\int d^2\mathbf{r}(\partial_\mu \hat{\mathbf{n}})^2$.

The general solution to (10) takes the form

$$\theta(r) = 2\tan^{-1}\left[(r/\rho_c)^{\mu s_1}\right], \tag{11}$$

where ρ_c is an arbitrary scale parameter which defines the core radius of the soliton. The validity of the continuum approximation, however, requires that $\rho_c \gg a$. Using condition (10), separation of variables is possible in polar coordinates for the set of eight, coupled, differential equations $H\tilde{\psi} = E\tilde{\psi}$, generated by the symmetrized form of the Hamiltonian operator (8). Defining the spatially nonvarying matrices $\alpha_\mu = U\tilde{\alpha}_\mu U^{+}$ and transformed wave function

$$\begin{aligned} \Psi = \sqrt{r} &\exp(is_1\gamma_x\sigma_z\pi/8) \\ &\times \exp(-is_1\sigma_z\phi/2) \exp(i\alpha_z\phi/2) U\tilde{\psi} \end{aligned} \tag{12}$$

leads, using the separability condition (10), to the new Schrödinger equation $H\Psi = E\Psi$ where

$$\begin{aligned} H = 2ita\left(\alpha_x\partial_r + \frac{\alpha_y}{r}(\partial_\phi + is_1\sigma_z/2)\right) + m\sigma_z\tau_z \\ -\mu\frac{ta}{r}[s_1 \sin\theta(r)\tau_x\sigma_y - \cos\theta(r)\sigma_z\alpha_y]. \end{aligned} \tag{13}$$

Some further simplifications emerge from the observation that the operators γ_x and $i\partial_\phi$ commute with this Hamiltonian and can be replaced by their eigenvalues $s_2 = \pm 1$ and $l = 0, \pm 1/2, \pm 1, \ldots$, respectively.

The energy levels corresponding to the localized gap solutions of this equation for topological charge $\mu = 1$ and $\mu = 2$ are shown in Fig. 2 as a function of the soliton core size ρ_c. For topological charge $\mu = 1$ it is necessary that $l \neq 0$ for the physical wave function to be nonsingular at the origin. Setting $s_1 = 1$ and $l = 1/2$ yields solid curve in Fig. 2. The bound state energy moves deeper into the Mott-Hubbard gap as the core radius ρ_c shrinks reaching a minimum value of approximately 0.75 the midgap energy. For topological charge $\mu = 2$ a nonsingular wave function may be obtained by setting $s_1 = 1$ and $l = 0$. The lowest bound state energy is depicted

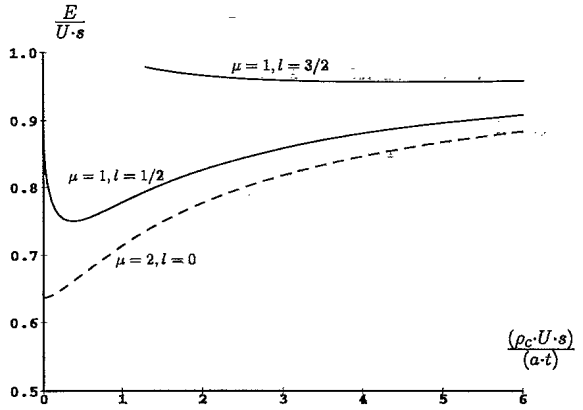

FIG. 2. Subgap electronic energy levels induced by hedgehog solitons of topological charge $\mu = 1$ (solid line) and $\mu = 2$ (dashed line) as a function of the dimensionless soliton core radius $(\frac{\rho_c}{a})(\frac{m}{t})$. $E/(Us) = 1$ and 0 are the upper band edge and midgap, respectively. Each level is doubly degenerate and the entire spectrum is symmetric under $E \rightarrow -E$.

by the dotted curve in Fig. 2. The energy eigenvalue decreases monotonically with decreasing ρ_c, approaching a limiting value of approximately 0.64 of the midgap as $\rho_c \rightarrow 0$. It is straightforward to prove that for any given state of energy E and angular momentum l, there is a corresponding state of energy $-E$ and angular momentum $-l$. Also, each level E is doubly degenerate. This arises from a sublattice degeneracy of the original square lattice. One state, with angular momentum l, resides primarily on one sublattice, whereas a degenerate state, with angular momentum $-l$, resides primarily on the other sublattice. In addition, a number of near band edge solutions appear for higher values of quantum number l. This leads to a possibility of electric-dipole allowed transitions at mid-infrared frequencies. For example, if $\delta > 0$, the $\mu = 1$ soliton exhibits an electronic transition between the states $(-E,\ l = 3/2)$ and $(-E,\ l = 1/2)$. In addition, there is a high frequency subgap transition from the state $(-E,\ l = 1/2)$ to $(+E,\ l = 3/2)$. A detailed derivation of these solutions and discussion of their properties will be presented elsewhere [15].

The possible existence of a topological many-electron condensate, and magnetic soliton excitations raises a number of important questions bearing on the anomalous normal state of high temperature superconductors. It is of particular importance to determine if, at finite doping, a topological condensate is energetically favored over the traditional spiral magnetic states described previously and if so whether a quantum liquid of solitons is responsible for the destruction of magnetic long-range order. Since the time scale of magnetic fluctuations is long compared to optical excitation time scales, it is plausible that a well defined subgap electronic structure exists even within a spin liquid phase. The interaction of these magnetic solitons with electrons near the Fermi surface need to be carefully investigated. This may in turn lead to new effective electron-electron interactions. In addition, the possibility of more general topological textures such as meron-meron configurations [17] which break cylindrical symmetry and the possibility of quantum number fractionalization need to be studied. It would indeed be remarkable if the unconventional properties of doped Mott insulators, including their high temperature superconductivity, could in this way be traced to the topological structure of the physical rotation group SO(3).

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