Solitons in Chiral-Spin Liquids

D. S. Rokhsar
Department of Physics, University of California, Berkeley, California 94720
(Received 13 July 1990)

We consider the low-lying states of a class of tight-binding models related to the parity- and time-reversal-breaking chiral-spin liquid, which describes a magnetically frustrated Mott insulator. In precise analogy with the soliton excitations of polyacetylene, the presence of a midgap state bound to topological disruptions of the chiral order leads to neutral, spin-$\frac{1}{2}$ spinons and charge-e, spinless holons.

PACS numbers: 71.30.+h, 75.10.Jm

"Resonating-valence-bond" (RVB) or "spin-liquid" scenarios for high-temperature superconductivity center on hypothesized Mott insulators composed of locally singlet-paired spins or "valence bonds."[1] Upon doping, it is supposed that these pairs maintain their integrity, and condense into a charge-$2e$ superconductor. It has been argued[2,3] that RVB insulators should support quasiparticles with reversed charge-spin relations: a spin-$\frac{1}{2}$, neutral "spinon" which is simply an unpaired spin immersed in the sea of paired spins, and a spinless, charge-e "holon" which is an unoccupied site amid the singlet fluid. Using this language, one hopes to develop a theory of the superconducting state as a dilute gas of holons which is complementary to a BCS-like description in terms of a dense fluid of paired electrons.

How can we reconcile this suggestion with the experimental fact that the undoped progenitors of high-temperature superconductivity display conventional Néel order? The answer lies in the fate of this order upon doping. With only a few percent charge carriers, the spin-correlation length plummets to a few lattice spacings.[4] Only then does superconductivity emerge, *after* long-range antiferromagnetic order has been obliterated. In addressing the nature of a Mott-insulator to superconductor transition, it therefore seems simplest to consider those Mott insulators whose spin correlations resemble the short-range correlations of a (gapped) singlet superconductor. The physical superconducting state can then be studied theoretically by turning on frustrating interactions, doping the resulting spin liquid, and finally turning off the artificially added frustration.

We consider here the low-lying spin- and charge-carrying excitations of an insulating spin liquid by studying the ground and relevant low-lying states of tight-binding models related to the parity- and time-reversal-breaking "chiral state."[5] It is argued that these states may be closely related to low-lying states of moderately frustrated Heisenberg models. We then present numerical evidence which supports the existence of spinons and holons, and discuss their interactions.

Local gauge symmetry and Mott insulators.— In terms of the underlying fermionic degrees of freedom, Mott insulators possess a local U(1) gauge symmetry,[6] since for energies small compared with the charge gap, the particle number on each site is conserved. Formally, a local gauge transformation $c_{i\alpha}^\dagger \rightarrow \exp(i\Lambda_i)c_{i\alpha}^\dagger$ simply multiplies every state in the singly occupied Hilbert space by the same overall phase factor $\exp(i\sum_i \Lambda_i)$ and therefore leaves all spin observables unchanged. Affleck and Marston[7] have proposed a mean-field theory which respects this gauge symmetry by reminding us that antiferromagnetic exchange arises from a virtual hop from site i to j and back again, viz., $-2J_{ij}(c_{i\alpha}^\dagger c_{j\alpha})(c_{j\beta}^\dagger c_{i\beta})$. This expression pleads for the introduction of the complex link variables $\chi_{ij} \equiv (J_{ij}/2)\langle c_{j\alpha}^\dagger c_{i\alpha}\rangle$ and the corresponding mean-field Hamiltonian

$$\mathcal{H}_{\rm MF} = \sum_{(i,j)} \frac{|\chi_{ij}|^2}{J_{ij}} + \sum_{(i,j)} \{\chi_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \text{H.c.}\} . \qquad (1)$$

From the definition of χ_{ij} we see that under a gauge transformation this effective hopping-matrix element acquires a phase factor $\exp[i(\Lambda_j - \Lambda_i)]$, so that Eq. (1) is gauge invariant. The mean-field ground state is obtained by minimizing $\mathcal{H}_{\rm MF}$ with respect to the χ_{ij}.

In general,[8] $\mathcal{H}_{\rm MF}$ is minimized by states with nonzero χ_{ij} only on isolated links of the lattice. The hypothesized spin liquids, however, are translationally invariant.[9] In a mean-field approximation, such states can be stabilized by the introduction of a biquadratic interaction,[7] which suppresses fluctuations of the magnitude $|\chi_{ij}|$. Alternately one may disregard these fluctuations by fiat, fixing $|\chi_{ij}|$ and allowing only the phases of χ_{ij} to vary. Either way, the Gutzwiller projections of these half-filled Slater determinants yield excellent variational energies[10] (and therefore accurately describe short-range correlations) when the "flux" through every elementary plaquette $ijkl$ is π, i.e., when $\chi_{ij}\chi_{jk}\chi_{kl}\chi_{li}$ is negative. On a square lattice with diagonal (frustrating) interactions, the optimal state (with uniform $|\chi_{ij}|$) is the chiral state,[5] with flux $\pi/2$ through each elementary triangle.

A weak-coupling approach.— In dealing with strongly interacting systems, one often relies on the principle of adiabatic continuity— the low-energy, long-wavelength properties of a system can be studied by tuning parameters to a more felicitous set of couplings as long as a phase boundary is not encountered. An instructive example of such a sequence of models is the half-filled, square-lattice Hubbard model with nearest-neighbor hopping.[11] In the small-Hubbard-U limit, this system is a commensurate spin-density-wave insulator, with an exponentially small charge gap. In the opposite large-Hubbard-U limit, charged excitations can be formally eliminated, resulting in a Heisenberg antiferromagnet. In both cases, the ground-state density correlations decay exponentially, and the low-energy, long-wavelength excitations are gapless antiferromagnons. Despite the apparent conceptual difference between a commensurate spin-density-wave insulator (whose charge gap is due to a doubled unit cell), and a Néel-ordered Mott insulator (whose gap is generally viewed as a many-body effect), there appears to be no phase boundary separating them.

Encouraged by the success of the weak-coupling approach to Néel-ordered insulators, we may ask if there exist tight-binding models whose ground and low-lying states smoothly interpolate from Slater determinants to spin-liquid states as repulsive interactions are turned on. In particular, we consider the extended Hubbard model in an arbitrary magnetic field,

$$\mathcal{H} = -\sum_{(i,j)} (T_{ij} e^{i\phi_{ij}} c_{i\alpha}^{\dagger} c_{j\alpha} + \text{H.c.}) + U \sum_i \tfrac{1}{2} n_i(n_i - 1) , \quad (2)$$

where $n_i = \sum_\alpha c_{i\alpha}^\dagger c_{i\alpha}$ is the particle number at site i, the T_{ij} are real and positive, and hopping is not limited to nearest neighbors. At half filling in the large-U limit, for *any* choice of link phases $\{\phi_{ij}\}$, this Hubbard model approaches a frustrated Heisenberg model in which the ratios J_{ij}/J_{kl} are simply $(T_{ij}/T_{kl})^2$. Each set of link phases then provides us with a one-parameter family of Hamiltonians which interpolates between a soluble ($U=0$) model and an intractable spin model. Sufficiently clever choices of phases may then allow us to infer properties of the large-U state from a careful study of tight-binding models. Note that for large but not infinite U, the effective Heisenberg model generically contains three-spin interactions,

$$\sum_{ijk} \frac{T_{ij} T_{jk} T_{ki}}{U^2} \sin(\Phi_{ijk}) \mathbf{S}_i \cdot \mathbf{S}_j \times \mathbf{S}_k , \quad (3)$$

where $\Phi_{ijk} \equiv \phi_{ij} + \phi_{jk} + \phi_{ki}$ is the flux through triangle ijk. These terms vanish in the Mott limit, but may act as infinitesimal symmetry-breaking fields if the ground state of the corresponding frustrated Heisenberg model breaks time reversal or parity.

Of course, exhibiting a continuous family of *models* does not ensure that the corresponding *states* will vary smoothly, since a phase transition could intervene. One prerequisite for the absence of a phase transition between the large- and small-U limits is that (a) both limiting states must have the same symmetry. For example, weakly frustrated square-lattice antiferromagnets are thought to have Néel-ordered ground states, so that we cannot expect the (paramagnetic) ground states of tight-binding models (2) with weak second-neighbor hopping to continue smoothly as U is increased. A second requirement for continuity between a small-U state and a Mott insulator is that (b) the small-U state must be locally neutral with a gap to charged excitations. This condition ensures that a metal-insulator transition does not interrupt the continuation process.

Which link phases ϕ_{ij} are most likely to permit continuation from a (paramagnetic) Slater determinant to a translationally invariant Mott insulator? The similarity between the generalized Hubbard model (2) and the mean-field theory (1) suggests distributions of flux which correspond to mean-field solutions with uniform magnitudes $|\chi_{ij}|$. The corresponding Slater determinant will then have spin correlations which should closely resemble those of its large-U cousin, facilitating a smooth interpolation between the two states. We also require a single-particle gap at $U=0$, to satisfy condition (b). To obtain a translationally invariant insulator, we further demand that the charge density be uniform and that the current on each link vanish. This latter condition is simply the statement that the expectation value of the Hamiltonian is stationary with respect to varying the link phases, which is automatically satisfied by choosing fluxes corresponding to a uniform-amplitude mean-field state.

On the two-dimensional square lattice with first- and second-neighbor hoppings T_1 and T_2, we will consider flux $\pi/2$ per triangle and π per plaquette, corresponding to the chiral state. By condition (a), we will therefore be considering the continuation of this $U=0$ state to a Mott insulator which breaks time reversal and parity. This state has a single-particle gap which, as in the case of a commensurate spin-density wave, has a simple single-particle interpretation: The presence of π flux per plaquette doubles the (magnetic) unit cell, and opens a "chiral gap" for nonzero second-neighbor hopping. In what follows, we will *assume* that (for sufficient frustration) this choice of phases permits a smooth interpolation of the ground state and certain simple low-lying states between large and small U. We will argue further that flux patterns in which the flux per triangle is $\pi/2$ *almost* everywhere describe Slater determinants which are continuously related to interesting excited states of the chiral-spin liquid, namely, holons and spinons. The static interactions (but neither the dynamics nor the statistics) of the excitations can then be inferred from simple tight-binding calculations, which we carry out on lattices of order of 200 sites. Before discussing these results, we present some simple heuristic arguments based on the minimization of (2) with respect to the link phases.

Some simple arguments.— Let us consider the simple system consisting of L noninteracting electrons on an L-site loop through which a variable flux Φ is passed. What value of Φ minimizes the total energy of the system? There are three cases to consider: When L is $6,10,14,\ldots,$ the minimum energy occurs at $\Phi=0$. When L is a multiple of 4, the energy of the loop can be lowered by opening a gap at the Fermi level, and the lowest energy corresponds to $\Phi=\pi$. The same considerations imply that the optimal flux for odd L is $\pm\pi/2$. On the full lattice, the problem of the optimal flux distribution is considerably more complicated, but the loop paradigm (and perhaps more than a little hindsight) suggests that we satisfy the shortest loops on the lattice. These short loops (i.e., triangles and quadrilaterals) presumably dominate the energetics of the lattice problem, since longer loops will overlap, and the energetic gains and costs from motion along these closed paths will interfere and largely cancel one another. Detailed calculations have confirmed these heuristic "rules" on a wide variety of lattices.[12]

The loop argument provides us with simple caricatures of the spinon and holon. For simplicity, consider a triangular lattice with nearest-neighbor hopping and the optimal flux of $\pi/2$ per triangle. (Extensions to other lattices are trivial.) To consider static charged excitations, we eliminate one site, x. Following the loop rules, we should readjust the fluxes to satisfy the shortest loops in the mutilated lattice. Far from x no adjustment is needed, but the triangles which previously included x have been eliminated; the shortest closed path involving the neighborhood of x is now the hexagon surrounding it. Originally, this hexagon was composed of six elementary triangles, and therefore enclosed a net flux of $6\times(\pi/2)\equiv\pi$. Our heuristic arguments suggest, however, that after x has been removed the flux through this hexagon should vanish. We now have a simple caricature of a static holon—a vacant site accompanied by an excess flux of π. If we restore the missing site as well as the electron which occupies it at half filling, the result is a spinon. The corresponding construction works equally well on a square lattice, as discussed in detail below.

A simple topological argument also suggests a connection between spin $\frac{1}{2}$ and an excess flux π in a chiral-spin liquid, by an extension of Laughlin's argument[3] for the existence of spinons. Consider a two-dimensional spin liquid with periodic boundary conditions in both directions, covering a torus. Since the torus is closed and orientable, the net flux passing through it is necessarily a multiple of 2π. On an even-site lattice, the local energetic preference for a flux of π through each plaquette is compatible with this global constraint. On an odd-site lattice, however, the topological constraint forces the system to accept an additional half-flux quantum over and above the energetically preferred flux. The odd-site insulator must also have a half-odd-integer total spin, since it contains an odd number of electrons. We show below that the excess spin and flux indeed bind to form a spinon.

Charge-conjugation symmetry.—The full lattice Hamiltonian (2) has charge-conjugation symmetry if each elementary triangle has flux $\pm\pi/2$, regardless of the hopping magnitudes $|T_{ij}|$. For then a gauge can be found such that the *inter*sublattice hopping-matrix elements are purely real while the *intra*sublattice hopping-matrix elements are purely imaginary. One then easily verifies that the tight-binding part of (2) anticommutes with the antilinear conjugation operator $\hat{\Upsilon}$ which is the composition of time reversal and a momentum boost by $\mathbf{Q}=(\pi,\pi)$:

$$\hat{\Upsilon}\sum_i \psi_i|i\rangle=\sum_i \psi_i^* e^{i\mathbf{Q}\cdot\mathbf{r}_i}|i\rangle\,. \tag{4}$$

Consequently, every single-particle eigenstate Ψ with energy E has a conjugate eigenstate $\hat{\Upsilon}\Psi$ with energy $-E$. This symmetry depends *only* on the phases ϕ_{ij} and *not* on the hopping magnitudes T_{ij}, and therefore applies to any lattice which can be considered a sublattice of a square (or hypercubic) lattice with $\pm\pi/2$ flux per triangle, such as a triangular lattice with flux $\pm\pi/2$ per triangle, a Kagome lattice with flux $\pm\pi/2$ per triangle and flux 0 or π per hexagon, etc. The ($U=0$) ground states of these models are obtained by filling the lower half of the spectrum. Since charge density (measured from half filling) and current are charge-conjugation odd, expectation values of these operators vanish in the ground state, as required in an insulator. A many-body charge-conjugation operator can also be defined[13] for nonzero values of U.

The chiral state.—The only translationally invariant, fully gapped state which satisfies the loop rules is the chiral state,[5] with flux $\pi/2$ per elementary triangle and π per plaquette. This state breaks parity and time reversal, since under either of these operations $\pi/2$ flux is transformed into $-\pi/2$ flux. The spin- and charge-correlation lengths in the $U=0$ chiral state are equal, with both roughly the larger of $|T_1/T_2|$ and $|T_2/T_1|$.

The chiral state possesses spin-1, momentum (π,π), particle-hole excitations corresponding to the transfer of an electron from an occupied lower band state Ψ to its upper band conjugate $\hat{\Upsilon}\Psi$, with a spin flip. The resulting exciton is neutral (by conjugation symmetry) and has a $U=0$ excitation energy equal to the chiral gap. We know that for small T_2/T_1 (corresponding to small J_2/J_1 in the large-U limit) the $U=0$ chiral state *cannot* continue smoothly to the large-U ground state of (2), since weak frustration does not destroy Néel order. As U is increased from zero in this regime, one therefore expects a critical U_c (of order of the chiral gap) above which long-range Néel order appears and the gap to spin-1 excitations collapses, as required by Goldstone's theorem. We now show that for $U=0$ and moderate T_2/T_1 the spin-1 exciton is unstable to decay into two spin-$\frac{1}{2}$ soliton excitations. This qualitative change in the nature of the low-lying spin excitations removes the natural mechanism for a transition to Néel order at large U.

Inhomogeneous states and spinons.—As noted above, it is impossible to construct a translationally invariant flux distribution which satisfies the loop rules on a periodic, odd-site lattice. The flux pattern which violates the fewest loop rules has flux $\pi/2$ through every triangle except for one "defective" triangle, which has flux $-\pi/2$, i.e., an additional half-flux quantum π passing through it. (This forces one plaquette to have no flux, violating the loop rules.) Numerically we find a spectrum whose density of states is essentially unchanged except for the appearance of a single, self-conjugate "midgap" state localized about the defective triangle. The half-filled ground state of the odd-site lattice is then obtained by filling the lower band and occupying the midgap state with a single electron. In precise analogy with the Su, Schrieffer, and Heeger[14] model for the spin soliton of polyacetylene, the resulting state is locally neutral and has spin $\frac{1}{2}$ localized within a spin-correlation length about the defective triangle. This is the one-spinon state.

Neutral spin-$\frac{1}{2}$ excitations can also be studied on even-site lattices by considering inhomogeneous chiral states with *two* defective triangles, each with an excess half-flux quantum. When these two triangles are far separated from one another, a conjugate pair of states appear in the gap. These midgap states are simply the bonding and antibonding combinations of the single localized state at each defect. Doubly occupying the bonding state corresponds to a singlet pair of spinons; occupying both bonding and antibonding states with spin-up electrons yields the $S^z=1$ component of a triplet spinon pair.

To address static interactions between spinons we must compare the energies of states with spinons at different separations. In the spirit of our approach, we make the additional assumption that the ordering of levels for different flux distributions at $U=0$ will be preserved upon continuation to the Mott limit.[15] In the singlet channel, one finds numerically that the interaction is attractive at all separations, so that a singlet spinon pair will annihilate. In both the singlet and triplet channels, the energy of a far separated pair of spinons is found to be simply twice the energy of a single spinon, confirming that spinons are not confined by a long-range potential. A qualitative change in the system, however, occurs for $T_2/T_1 > 0.25$, when the energy of a triplet spinon pair crosses below the energy of the spin-1 exciton of the uniform chiral state discussed previously. Spinons then become the lowest-energy spin excitations.

Static holes and holons.—The small-U approach to Mott insulators is easily extended to encompass static holes, since these are vacancies in the lattice and local gauge invariance remains. If we eliminate one site from an even-by-even lattice, the resulting spectrum possesses an odd number of states. Charge conjugation then demands a midgap state, which is localized near the missing site. When all remaining sites of the lattice are half filled, the ground state is given by filling the valence band and singly occupying the midgap state. In this case, the resulting wave function corresponds to a charge-e, spin-$\frac{1}{2}$ hole (*not* a holon), with the charge contributed by the absent site and the spin contributed by the localized midgap electron.

We may also consider an odd-by-odd lattice with a deleted site pierced by an excess half-flux quantum, as suggested by our earlier heuristic arguments. There are then an even number of states, and hence no midgap level; the ground state is simply a filled valence band. This is a holon wave function with charge e and spin 0, the precise analog of the charged soliton in polyacetylene.

Again assuming that the ordering of levels is maintained[15] between small and large U, we find numerically that a static hole is more stable than a static, far separated spinon-holon pair. As in polyacetylene, an energy of order the chiral gap is needed to separate spin and charge, but two isolated, static charged solitons are more stable than two isolated, static holes. Unlike polyacetylene, however, a pair of holons *attract* one another, forming a bound state which is indistinguishable from a two-*hole* bound singlet pair. It will be argued elsewhere that a superconductor obtained by Bose condensation of these pairs has time-reversal- and parity-noninvariant d-wave symmetry with a full energy gap.

I thank Daniel Fisher, Steve Kivelson, Dung-Hai Lee, and Brad Marston for many interesting discussions. This work was supported by National Science Foundation Grant No. DMR 89-14440.

[1]P. W. Anderson, Science **235**, 1196 (1987).

[2]S. Kivelson, D. S. Rokhsar, and J. P. Sethna, Phys. Rev. B **35**, 8865 (1987).

[3]V. Kalmeyer and R. B Laughlin, Phys. Rev. Lett. **59**, 2095 (1987); R. B. Laughlin, Science **242**, 525 (1988).

[4]R. J. Birgenau *et al.*, Phys. Rev. B **38**, 6614 (1988).

[5]X. G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B **39**, 11413 (1989).

[6]G. Baskaran and P. W. Anderson, Phys. Rev. B **37**, 580 (1989).

[7]I. Affleck and J. B. Marston, Phys. Rev. B **37**, 3774 (1988); J. B. Marston and I. Affleck, *ibid.* **39**, 11538 (1989).

[8]D. S. Rokhsar, Phys. Rev. B **42**, 2526 (1990).

[9]Numerical studies of frustrated spin-$\frac{1}{2}$ Heisenberg models suggest that Néel order is destroyed for sufficient frustration, but the nature of the ground states remains unclear. See, e.g., E. Dagotto and A. Moreo, Phys. Rev. B **39**, 4744 (1989); F. Figuerido *et al.*, Phys. Rev. B **41**, 4619 (1990).

[10]C. Gros, Phys. Rev. B **38**, 931 (1988).

[11]J. R. Schrieffer, X. G. Wen, and S.-C. Zhang, Phys. Rev. B **39**, 11663 (1988).

[12]J. B. Marston and D. S. Rokhsar (unpublished).

[13]S. Kivelson and W.-K. Wu, Phys. Rev. B **34**, 5423 (1986).

[14]W. P. Su, J. R. Schrieffer, and A. Heeger, Phys. Rev. Lett. **42**, 1698 (1979).

[15]By working with static solitons we are neglecting their (not necessarily small) delocalization energies.