Large-U limit of a Hubbard model in a magnetic field: Chiral spin interactions and paramagnetism

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We consider the large-U limit of the one-band Hubbard model at half-filling on a nonbipartite two-dimensional lattice. An external magnetic field can induce a three-spin chiral interaction at order $1/U^2$. We discuss situations in which, at low temperatures, the chiral term may have a larger effect than the Pauli coupling of electron spins to a magnetic field. We present a model that explicitly demonstrates this. The ground state is a singlet with a gap; hence the spin susceptibility is zero while the chiral susceptibility is finite and paramagnetic.

The ground-state and low-energy excitations of Heisenberg antiferromagnets have been extensively studied in recent years. One reason for this interest is that the simplest model for strongly correlated electron systems, the one-band Hubbard model, reduces at half-filling to a Heisenberg antiferromagnet in the limit of large on-site Coulomb repulsion U.[1] Specifically, the Hubbard Hamiltonian is

$$H = -\sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} , \qquad (1)$$

where $t_{ij} = t^*_{ji}$ is the hopping integral from site j to site i, and $\sigma = \pm 1$ or, equivalently, $\uparrow$ and $\downarrow$, and $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$. At half-filling, $\sum_{i,\sigma} n_{i\sigma}$ is equal to the number of sites. In the large-U limit, the low-energy subspace of the total Hilbert space consists of states with exactly one electron at each site. To order $1/U$, this subspace is governed by the spin Hamiltonian

$$H_{sp} = \sum_{ij} J_{ij} \frac{\mathbf{S}_i \cdot \mathbf{S}_j}{\hbar^2} . \qquad (2)$$

Here $\mathbf{S}_i = (\hbar/2) c^{\dagger}_{i\sigma} \tau_{\sigma\sigma'} c_{i\sigma'}$, with τ being Pauli spin matrices (the indices σ and σ' are summed over). The couplings $J_{ij} = 2|t_{ij}|^2/U$ are antiferromagnetic. At higher orders in $1/U$, J_{ij} are renormalized and multispin interactions appear in $H_{\rm sp}$. These can be calculated as an expansion in t_{ij}/U by relating Eqs. (1) and (2) through a unitary transformation.[2]

In this paper, we examine what happens when this model is placed in a magnetic field.[3] The application of the field has two effects. First, the t_{ij} pick up a phase $\exp[(ie/c\hbar)\int_i^j \mathbf{A}\cdot d\mathbf{r}]$, where $\mathbf{A}$ is the vector potential. Hence the phase of the string $t_{ij} t_{jk} \cdots t_{ki}$ connecting three or more sites forming a closed curve is proportional to the flux enclosed by that curve. Second, there is the Pauli interaction given by $\nu \mathbf{S}_i \cdot \mathbf{B}/\hbar$, where $\nu = -e\hbar/mc$, with $e(m)$ and c denoting the charge (mass) of the electron and the velocity of light, respectively. (As explained below, the Pauli term takes the same form in the Hubbard and spin Hamiltonians.) We are interested in finding out whether the phases in t_{ij} induce any unusual terms in $H_{\rm sp}$, and what effects such terms may have. Since an external magnetic field breaks invariance under time reversal T, we might expect $H_{\rm sp}$ to reflect this. That is, if $\mathbf{B} \to -\mathbf{B}$ so that $t_{ij} \to t^*_{ij}$, there should be terms in $H_{\rm sp}$ which reverse sign. It turns out that no T-violating terms are induced in $H_{\rm sp}$ on bipartite lattices, as one can show by using the particle-hole symmetry at half-filling. We transform $c_{i,\sigma} \to \sigma c^{\dagger}_{i,-\sigma}$ on the sites of one sublattice, and $c_{i,\sigma} \to -\sigma c^{\dagger}_{i,-\sigma}$ on the other sublattice. This is a symmetry of (1) if $t_{ij} \to t^*_{ij}$ at the same time. Since $\mathbf{S}_i$ remains invariant under this transformation, $H_{\rm sp}$ must be the same for $\mathbf{B}$ and $-\mathbf{B}$. So the T violation appears to lie entirely in the high-energy subspace (states with one or more doubly occupied sites) for bipartite lattices. We also observe that on *any* lattice, particle-hole symmetry implies that $H_{\rm sp}$ must remain invariant if $t_{ij} \to -t_{ji}$ in (1). Hence if the t_{ij}'s are all real, $H_{\rm sp}$ cannot have odd powers of t_{ij}.

We must therefore consider nonbipartite lattices to obtain something interesting. The simplest example consists of three sites i, j, and k forming a triangle. The perturbative expansion in t_{ij}/U is obtained by first writing the hopping term in (1) as the sum of three terms T_0, T_1 and $T_{-1} = T^{\dagger}_1$, where T_m increases the number of doubly occupied sites by m when it acts on a state.[2] The unitary operator relating (1) and (2) is then given by $\exp[iK]$, where K is a power series in T_m/U. (Note that the Pauli interaction commutes with all the T_m's and therefore with K.) At half-filling, the low-energy subspace (states with no doubly occupied sites) is annihilated by both T_0 and T_{-1} since any hopping necessarily takes us to a state with one doubly occupied site. We then find that

$$H_{\rm sp} = \frac{\nu}{\hbar} \sum_i \mathbf{S}_i \cdot \mathbf{B} - \frac{1}{U} T_{-1} T_1 + \frac{1}{U^2} T_{-1} T_0 T_1 . \qquad (3)$$

When rewritten in the language of spin-$\frac{1}{2}$ operators, the second term on the right-hand side of (3) is the same as Eq. (2), while the third term is a three-spin chiral interaction[3] of the form $\mu \mathbf{S}_i \cdot \mathbf{S}_j \times \mathbf{S}_k / \hbar^3$, where

$$\mu = \frac{24}{U^2} \mathrm{Im}(t_{ij} t_{jk} t_{ki}) \ . \tag{4}$$

This vanishes if the t_{ij}'s are real. Let the magnetic flux enclosed by the triangle be Φ. If we denote the magnitude $|t_{ij} t_{jk} t_{ki}| \equiv t^3$ for simplicity, then

$$\mu = \frac{24t^3}{U^2} \sin \left[\frac{e\Phi}{c\hbar} \right] . \tag{5}$$

One can estimate the relative magnitudes of this chiral term and the Pauli term for some typical values of t_{ij}, U, and the area of the triangle A.[4] For $A = 2$ Å^2, the number $e\Phi / c\hbar$ is much smaller than 1 unless the field B reaches the fantastically large value of 10^4 T. Hence we replace the sine in Eq. (5) by its argument, so that

$$\mu = \frac{24t^3}{U^2} \frac{eA}{c\hbar} B \cos\theta \ , \tag{6}$$

where θ is the angle between $\mathbf{B}$ and the normal to the plane of the triangle. We then find that for $t = 0.5$ eV and $U = 5$ eV, the magnitude of the Pauli term is about 40 times larger than the chiral term. This estimate follows from comparing the splitting in the ground-state energy produced by the Pauli and chiral interactions for a triangle in which the three J_{ij}'s are equal. That is, we take the Hamiltonian on a triangle to be

$$H_{\rm sp} = J[\mathbf{S}_i \cdot \mathbf{S}_j + \mathbf{S}_j \cdot \mathbf{S}_k + \mathbf{S}_d \cdot \mathbf{S}_i] + \frac{\mu}{\hbar^3} \mathbf{S}_i \cdot \mathbf{S}_j \times \mathbf{S}_k + \frac{\nu}{\hbar} (\mathbf{S}_i + \mathbf{S}_j + \mathbf{S}_k) \cdot \mathbf{B} \ . \tag{7}$$

If $\mathbf{B} = 0$, the ground state of this Hamiltonian has a fourfold degeneracy with all states having total $S = \frac{1}{2}$. The magnetic field breaks this degeneracy completely with the Pauli and chiral terms contributing $\pm \nu B / 2$ and $\pm \sqrt{3} \mu / 4$, respectively. For the excited states with $S = \frac{3}{2}$, we observe that the chiral term has no effect. Thus the chiral interaction can only lower the energy of a state if it is nonferromagnetic.

Although the Pauli term appears to be numerically much larger than the chiral term, one can think of two possible situations in which the chiral interaction dominates. The first example is one in which the ground state is a spin singlet and is chiral *even* in the absence of the magnetic field. We have in mind here the two-dimensional models discussed by Wen, Wilczek, and Zee[5] where a spin Hamiltonian has two degenerate singlet ground states with opposite chiralities. We can say that each ground state has a nonzero chiral moment M_c (defined below). Then an applied magnetic field picks out one of the two ground states due to an interaction of the form $-M_c B$. The Pauli term $\mathbf{S} \cdot \mathbf{B}$ (where $\mathbf{S} = \sum_i \mathbf{S}_i$) plays no role here because the ground states are singlets. However, these kinds of models often require a special choice of the two-spin couplings J_{ij} as well as peculiar multispin interactions in order to produce the required ground-state degeneracy. There are also papers which argue that frustrated antiferromagnets with only two-spin interactions can have chiral ground states.[5–7] However, this has been questioned,[8] and it seems to be quite difficult to have chiral ground states in the absence of an external magnetic field.

The second example, which has only short-range two-spin interactions and does not require a fine tuning of the couplings, is one in which the ground state is a singlet, unique and nonchiral in the absence of the magnetic field. Further, there is a gap Δ to states with total spin greater than zero. Then the ground state continues to be a singlet in the presence of a field if $|\nu B| \ll \Delta$. But it may develop a chiral moment M_c to first order in B, and one can define a chiral susceptibility $\chi_c \equiv (\partial M_c / \partial B)_{B=0}$. So one may have a finite χ_c even though the spin susceptibility $\chi_s = \partial \langle S \rangle / \partial B = 0$. We now present a two-dimensional model which explicitly demonstrates all this. Incidentally, it is the only two-dimensional spin model that we are aware of in which the ground state and the low-lying excitations can be found exactly (for the Hamiltonian H_0 given below).

Our model, shown in Fig. 1, consists of chains of rhombuses which are coupled to each other in the form of a brick lattice. Each rhombus is formed out of two triangles with a common base. The number of rhombuses is $N/3$ if the number of sites is N. Starting from a Hubbard model with only nearest-neighbor hoppings, the spin Hamiltonian in a magnetic field is given up to order $1/U^2$ by

$$H_{\rm sp} = H_0 + \mu \frac{C}{\hbar^3} \ , \tag{8}$$

where

$$H_0 = \sum_{ij} J_{ij} \frac{\mathbf{S}_i \cdot \mathbf{S}_j}{\hbar^2} + \frac{\nu}{\hbar} \sum_i \mathbf{S}_i \cdot \mathbf{B}$$

and

$$C = \sum_\alpha \mathbf{S}_3 \cdot \mathbf{S}_4 \times (\mathbf{S}_2 - \mathbf{S}_5) \ .$$

The chiral term C is a sum over rhombuses labeled by the index α, with each rhombus contributing the sum of two three-spin terms as indicated in Eq. (8). (See Fig. 1 for the site labels 1–6 in and around a typical rhombus.) Note that the Pauli term has been included in an unperturbed Hamiltonian H_0, while the chiral term will be considered perturbatively in the following. If we define

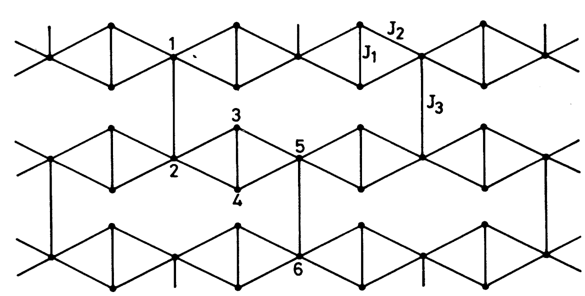

FIG. 1. The model showing six sites labeled 1–6 in and around a typical rhombus. The three different antiferromagnetic couplings J_1, J_2, and J_3 are also indicated.

parity to be the transformation which exchanges the top and bottom sites of the vertical bonds inside all the rhombuses simultaneously (namely, $3 \leftrightarrow 4$ in the figure), then C is odd under parity while H_0 is even under parity.

In H_{sp}, the couplings J_{ij} on the vertical bonds inside the rhombuses, the slanted bonds, and the vertical bonds joining the chains are denoted by J_1, J_2 and J_3, respectively, as shown in Fig. 1. Let us assume that $J_1 > 2J_2$ and that $|\nu B|$ is much less than both $(J_1 - 2J_2)\hbar$ and $J_3\hbar$. Then one can prove that the ground state of H_0 is a singlet, unique, and has a gap Δ_0 to all excitations. Let us first introduce the notation O_{ij} and 1_{ij} for the singlet and triplet states, respectively, formed from the spins at sites i and j. Note that $O_{ij} = 1/\sqrt{2}(|i\uparrow j\downarrow\rangle - |i\downarrow j\uparrow\rangle)$ is antisymmetric under an exchange of i and j, while the three states collectively denoted by 1_{ij} are all symmetric. Then the ground state of H_0 is the state ψ_0 given by the product of singlets $\ldots O_{12} \otimes O_{34} \otimes O_{56} \ldots$ following the labels in Fig. 1. That is, each of the vertical bonds form a singlet. The ground-state energy is $E_0 = -(N/8)(2J_1 + J_3)$.

To prove that ψ_0 is the ground state and that there is a gap Δ_0, let us write $H_0 = H_1 + H_2$, where H_1 is the same as H_0 except that the couplings J_1 are replaced by $J_1 - 2J_2$ and the couplings J_2 are replaced by zero. Thus H_1 is a sum of disconnected two-spin Hamiltonians involving only the vertical bonds, while H_2 is a sum of disconnected four-spin Hamiltonians of the form $(J_2/2)[(\mathbf{S}_2+\mathbf{S}_3+\mathbf{S}_4)^2 + (\mathbf{S}_3+\mathbf{S}_4+\mathbf{S}_5)^2]$ for each rhombus. It is then easy to find the complete spectra for both H_1 and H_2. For H_1, ψ_0 is the unique ground state and there is a finite gap $\Delta_1 = \min(J_1 - 2J_2 - |\nu B|, J_3 - |\nu B|)$ to the space of states orthogonal to ψ_0. For H_2, ψ_0 is a ground state but there is no gap to its orthogonal subspace. It then follows that ψ_0 is the ground state of $H_1 + H_2$ and there is a gap $\Delta_0 \geq \Delta_1$ to all other states.[9] We also note that the total spin on any bond of type J_1 [e.g., $(\mathbf{S}_3+\mathbf{S}_4)^2$] commutes with H_0, so that there are $N/3$ operators which can be diagonalized along with H_0. This important property proves to be very useful. For instance, it implies that a low-lying excitation can only have a *finite* number p of J_1 bonds forming triplets. [Such a state is separated from the ground state by a gap $\Delta \geq p(J_1 - 2J_2 - |\nu B|)$ by a similar argument involving H_1 and H_2]. Further, such an excitation can only differ from the ground state in a local neighborhood of those p triplet bonds or due to some isolated J_3 bonds forming triplets instead of singlets. Hence all low-lying excitations are localized and dispersionless (with energy independent of the momentum).

One can check that ψ_0 is nonchiral; that is, $\langle \psi_0 | C | \psi_0 \rangle = 0$. The simplest way to show this is to write $C = \sum_\alpha C_\alpha$, where C_α is the sum of the two chiral terms in a rhombus α. Consider the rhombus made out of sites 2, 3, 4, and 5 in Fig. 1. Both ψ_0 and C_α for that rhombus are odd under the parity transformation $3 \leftrightarrow 4$. Hence $C_\alpha|\psi_0\rangle$ is even under parity, i.e., it contains 1_{34} rather than O_{34}. Hence $\langle \psi_0 | C_\alpha | \psi_0 \rangle$ must be zero. We will now assume that the term μC in (8) only changes the ground state perturbatively because we expect the gap to survive for a finite range of μ around $\mu = 0$. We can therefore use second-order perturbation theory to compute the ground-state energy $E_0(\mu)$ to order μ^2. Since μ is proportional to B, this will give us the chiral moment $M_c \equiv -\partial E_0(\mu)/\partial B$ and the chiral susceptibility $\chi_c = \partial M_c / \partial B$.

The second-order expression is

$$E_0(\mu) - E_0 = \mu^2 \sum_{n \neq 0} \sum_{\alpha,\beta} \frac{(C_\alpha)_{0n}(C_\beta)_{n0}}{E_n - E_0} , \tag{9}$$

where $(C_\alpha)_{mn} = \langle \psi_m | C_\alpha | \psi_n \rangle$ and m and n label the eigenstates of H_0. Now we know that the state $C_\beta|\psi_0\rangle$ has the J_1 bond in rhombus β forming a spin triplet, while the J_1 bonds in all other rhombuses are singlets. This implies that all the terms in (9) with $\alpha \neq \beta$ must vanish. Next let us consider a particular rhombus labeled β and the six sites in and around that rhombus as labeled in Fig. 1. Then $(C_\beta)_{n0}$ can only be nonzero for a *finite* number of states ψ_n since the singlet subspace of those six spins is five dimensional. Also, $(C_\beta)_{n0}$ can be nonzero only if the vertical bond in the rhombus β is a triplet in the state ψ_n. An explicit calculation shows that $(C_\beta)_{n0}$ is actually nonzero for only two states for which $E_n - E_0$ are given by

$$E_\pm - E_0 = J_1 - J_2 + \tfrac{3}{2}J_3 \pm \left[J_2^2 + \frac{J_3^2}{4} \right]^{1/2} , \tag{10}$$

respectively. ($E_\pm$ and E_0 are independent of the magnetic field B since all the states being considered are spin singlets.) We eventually find that

$$E_0(\mu) - E_0 = -\frac{N}{8}\mu^2 \frac{J_1 - J_2 + 2J_3}{(E_+ - E_0)(E_- - E_0)} . \tag{11}$$

This is of order t^4/U^3 since the couplings $J_{ij} \sim t^2/U$. This and Eq. (6) yield a paramagnetic susceptibility

$$\chi_c = \frac{N}{4} \left[\frac{24t^3}{U^2} \frac{eA}{c\hbar} \cos\theta \right]^2 \frac{J_1 - J_2 + 2J_3}{(E_+ - E_{-0})(E_- - E_0)} \tag{12}$$

to order t^4/U^3.

We emphasize that (11) is not the complete expression for the ground-state energy to order $1/U^3$, since we have ignored terms of order $1/U^3$ in deriving H_{sp} in (8). These terms do contribute to the energy in first-order perturbation theory. However, one can show that these terms are not chiral because they are even under parity. They are independent of μ and hence do not contribute to the chiral quantities M_c and χ_c to order t^4/U^3.

At finite temperatures, this model no longer has $\chi_s = 0$. But if the temperature is small compared to the gap, then χ_c will continue to be much larger than χ_s.

Our model is somewhat peculiar in that the two-spin correlation in the ground state of H_0 is *exactly* zero beyond a short distance. However, this property is unlikely to survive once we take into account the chiral terms and higher-order terms in $1/U$ which couple spins on non-neighboring sites. We then expect the two-spin correlation to go to zero exponentially at large separations because of the gap above the ground state. The ground state is therefore a spin liquid which is dominated by short-range valence bonds.

More realistic models which do not have a gap to spin excitations will generally have both χ_c and χ_s nonzero even at zero temperature. For instance, one can consider a Hubbard model on a triangular lattice, or on a square lattice with both nearest-neighbor and next-nearest-neighbor hoppings. Whether χ_c will be comparable to or much smaller than χ_s will then depend on the properties of low-energy excitations in the absence of the magnetic field. For instance, if there are singlet chiral states lying very close to a nonchiral ground state, then one would expect χ_c to be large. An important (and perhaps experimentally observable) difference between the two susceptibilities is that χ_c depends on the orientation of the magnetic field with respect to the plane containing the sites of the spins.

To conclude, we have seen that a spin system which arises from an underlying Hubbard model can develop chiral interactions when placed in a magnetic field. Although these interactions are small, they may lead to an interesting low-temperature phase resembling a chiral spin liquid.

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[1]P. W. Anderson, Science **235**, 1196 (1987); Phys. Rev. **115**, 2 (1959).

[2]A. H. MacDonald, S. M. Girvin, and D. Yoshioka, Phys. Rev. B **37**, 9753 (1988); C. Gros, R. Joynt, and T. M. Rice, *ibid.* **36**, 381 (1987); J. E. Hirsch, Phys. Rev. Lett. **54**, 1317 (1985); M. Takahaski, J. Phys. C **10**, 1289 (1977).

[3]D. S. Rokhsar, Phys. Rev. Lett. **65**, 1506 (1990); J. K. Freericks, L. M. Falicov, and D. S. Rokhsar, Phys. Rev. B **44**, 1458 (1991).

[4]P. W. Anderson, G. Baskaran, Z. Zou, and T. Hsu, Phys. Rev. Lett. **58**, 2790 (1987).

[5]X. G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B **39**, 11 413 (1989).

[6]V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987).

[7]G. Baskaran, Phys. Rev. Lett. **63**, 2524 (1989); I. Ritchey, P. Chandra, and P. Coleman, *ibid.* **64**, 2583 (1990); G. Baskaran, *ibid.* **64**, 2584 (1990).

[8]E. T. Tomboulis, Phys. Rev. Lett. **68**, 3100 (1992); S. Yu, Khlebnikov, Pis'ma Zh. Eksp. Teor. Fiz. **53**, 87 (1991) [JETP Lett. **53**, 88 (1991)]; E. Dagotto and A. Moreo, Phys. Rev. Lett. **63**, 2148 (1989).

[9]P. W. Anderson, Phys. Rev. **83**, 1260 (1951).