PHYSICAL REVIEW B VOLUME 41, NUMBER 16 1 JUNE 1990

Stability of the saturated ferromagnetic state in the one-band Hubbard model

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(Received 5 January 1990; revised manuscript received 8 May 1990)

We discuss the stability of the saturated ferromagnetic state of the one-band Hubbard model against a single spin flip in the limit of infinite on-site repulsion. We consider the case where the number of holes N_h can be large but satisfies the condition $N_h \ll \ln N$, in two dimensions, ($N_h \ll N^{1/3}$ in three dimensions) where N is the number of spins. We show that the Nagaoka state is locally stable, except for certain small values of N_h for which there is an instability at long wavelengths.

Our understanding of itinerant ferromagnetism is poor despite extensive work over many years.[1] Real itinerant ferromagnets, such as Fe and Ni have degenerate orbitals with (ferromagnetic) Hund's rule couplings between them. It is interesting to ask whether such couplings are vital to the stability of ferromagnetism in itinerant systems or not. In particular, it is not known for sure whether the one-band Hubbard model,[2] which cannot, of course, have such couplings, has a ferromagnetic phase.[3] Interest in this model recently has revived because of its possible relevance to high-temperature superconductivity[4] and this has led to new work on the older question of ferromagnetism.[5-8] The only rigorous result in this area is that of Nagaoka,[9] who showed that the ground state of one hole in the Hubbard model with infinite on-site repulsion, U, is a fully aligned ferromagnet, which we shall call the Nagaoka state. The interesting question is, of course, whether the system is ferromagnetic for a finite *density* of holes in the thermodynamic limit. In this paper we make a step towards answering this question by computing the local stability of the saturated ferromagnetic state (Nagaoka state) of the infinite-U Hubbard model with respect to a single spin flip, when the number of holes is large, but still less than a finite fraction of the number of sites.

Extrapolation of results on finite-sized systems to the thermodynamic limit is complicated by the irregular behavior observed[5-8] as a function of the number of holes. In this paper we try to make sense of this irregular behavior by studying, through a combination of analytical and numerical techniques, the case where the number of holes, N_h, satisfies the condition $N_h \ll \ln N$, where N is the number of sites on the two-dimensional square lattice. When this condition is fulfilled the spin-wave energy that we calculate is the excited state of *lowest energy*. The analogous condition in three dimensions is $N_h \ll N^{1/3}$. For larger numbers of holes the spin wave lies in a particle-hole continuum and the analysis is more complicated. Within these limits we show (i) that the finite-size corrections are large, (ii) for finite N_h, the spin-wave energy depends on whether or not the saturated ferromagnetic state has orbital degeneracy, (iii) for boundary conditions with nondegenerate Nagaoka state, the spin-wave energies are all positive and, at each wave-vector $\mathbf{Q}$, are proportional to the number of holes, (iv) for boundary conditions with a degenerate Nagaoka state, the spin-wave energies form several bands, the lowest of which has energy proportional to the number of holes in the *filled shells*, N_f, of the Nagaoka state, except for modes with $\mathbf{Q}$ close to zero, where (v) we find that the spin-wave energies are all positive, except that for certain finite values of N_h a small number of long wavelength modes are unstable. Note that our calculation is applicable to an infinite number of holes in the thermodynamic limit, though unfortunately not where N_h is a finite fraction of N. We now discuss briefly the model and calculational methods. A full account will be published separately.[10]

In the limit of infinite on-site repulsion the Hubbard model reduces to a problem of constrained hopping with the Hamiltonian given by

$$H = -t \sum_{\langle \mathbf{n},\mathbf{m}\rangle \sigma} (\tilde{c}^{\dagger}_{\mathbf{n}\sigma} \tilde{c}_{\mathbf{m}\sigma} + \tilde{c}^{\dagger}_{\mathbf{m}\sigma} \tilde{c}_{\mathbf{n}\sigma}) , \tag{1}$$

where $\langle \mathbf{n},\mathbf{m}\rangle$ indicates nearest-neighbor pairs, $\tilde{c}_{\mathbf{m}\sigma} = c_{\mathbf{m}\sigma} \times (1 - n_{\mathbf{m},-\sigma})$, $c^{\dagger}_{\mathbf{m}\sigma}$, $c_{\mathbf{m}\sigma}$ are the creation and annihilation operators of an electron in the site $\mathbf{m}$, and $n_{\mathbf{m}\sigma} = c^{\dagger}_{\mathbf{m}\sigma} c_{\mathbf{m}\sigma}$. Unless otherwise stated, our results will be for a square lattice with $N = L^2$ sites and periodic boundary conditions, but we will also comment on the analogous results for other boundary conditions and the simple cubic lattice, where appropriate. From now on, we set $t = 1$.

We confine our attention to the case of a single spin flip. Denoting by $\phi(\mathbf{Q};\mathbf{k}_1,\ldots,\mathbf{k}_{N_h})$, the amplitude to have the holes in states with wave vectors $\mathbf{k}_1,\ldots,\mathbf{k}_{N_h}$ and the spin flip to have wave vector $\mathbf{Q} - \sum \mathbf{k}_i$, the Schrödinger equation is found to be[9]

$$\left[\omega(\mathbf{Q}) - \sum_{i=1}^{N_h} \varepsilon(\mathbf{k}_i) + \sum_{i=1}^{N_h} \varepsilon(\mathbf{p}_i)\right] \phi(\mathbf{Q};\mathbf{k}_1,\ldots,\mathbf{k}_{N_h})$$
$$= \frac{1}{N} \sum_{\mathbf{k}'} \left[\varepsilon\left(\mathbf{k}' + \sum_{i=1}^{N_h} \mathbf{k}_i - \mathbf{Q}\right) - \varepsilon(\mathbf{k}')\right] [\phi(\mathbf{Q};\mathbf{k}',\mathbf{k}_2,\ldots,\mathbf{k}_{N_h}) + \phi(\mathbf{Q};\mathbf{k}_1\mathbf{k}',\ldots,\mathbf{k}_{N_h}) + \cdots + \phi(\mathbf{Q};\mathbf{k}_1,\ldots,\mathbf{k}')] , \tag{2}$$

with $\varepsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y)$. The energy $\omega(\mathbf{Q})$ is measured relative to that of the saturated ferromagnetic state, $\varepsilon_F = \sum \varepsilon(\mathbf{p}_i)$, where the $\{\mathbf{p}_i\}$, $i = 1, \ldots, N_h$, are the momenta of the holes in the Nagaoka state. The wave function $\phi(\mathbf{Q};\mathbf{k}_1, \ldots, \mathbf{k}_{N_h})$ must be completely antisymmetric in $\mathbf{k}_1, \ldots, \mathbf{k}_{N_h}$, and because of the constraint of no double occupancy, must satisfy $\sum_{\mathbf{k}'} \phi(\mathbf{Q};\mathbf{k}', \mathbf{k}_2, \ldots, \mathbf{k}_{N_h}) = 0$ for each $\mathbf{k}_2, \ldots, \mathbf{k}_{N_h}$. We have, for convenience, shifted all the wave vectors by (π,π), so that the wave vectors of the holes in the Nagaoka state, $\{\mathbf{p}_i\}$, are close to (0,0). This means that for an odd number of holes, the crystal momentum is actually not $\mathbf{Q}$ but $\mathbf{Q} - (\pi,\pi)$.

For the majority of hole numbers, the Nagaoka state is degenerate when one imposes periodic boundary conditions. We shall show that this degeneracy, which does not seem to have been treated analytically before, *does* affect the results for finite clusters, though it has a negligible effect when *both* N_h and N are large. A particular Nagaoka state Γ is specified by the set of wave vectors $\{\mathbf{p}_\mu\}$, $\mu = 1, \ldots, N_h$, which are occupied by holes. The degeneracy arises, of course, from the last shell being only partially filled. Let us denote by $\mathbf{p}_\alpha$, $\alpha = 1, \ldots, N_f$, a hole in a filled shell and by $\mathbf{p}_i$, $i = 1, \ldots, N_u$, a hole in the partially filled shell. Clearly we have $N_f + N_u = N_h$. As found by Nagaoka[9] and discussed further below, we need only consider states where, at most, only one hole is excited out of the Nagaoka state. Hence we define,

$$\phi_0^\Gamma = \phi(\mathbf{Q};\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_{N_h}) , \tag{3a}$$

$$\phi_i^\Gamma(\mathbf{p}_\mu, \mathbf{k}) = \phi(\mathbf{Q};\mathbf{p}_1, \ldots, \mathbf{p}_{\mu-1}, \mathbf{k}, \mathbf{p}_{\mu+1}, \ldots, \mathbf{p}_{N_h}) . \tag{3b}$$

Ignoring certain terms which are negligible in the thermodynamic limit, we find

$$\omega(\mathbf{Q})\phi_0^\Gamma = \frac{1}{N}\sum_{\alpha=1}^{N_f}[\varepsilon(\mathbf{p}_\alpha + \mathbf{P}_\Gamma - \mathbf{Q}) - \varepsilon(\mathbf{p}_\alpha)]\phi_0^\Gamma + \frac{1}{N}\sum_{i=1}^{N_u}\sum_j [\varepsilon(\mathbf{p}_j + \mathbf{P}_\Gamma - \mathbf{Q}) - \varepsilon(\mathbf{p}_j)](-1)^{l_{ij}}\phi_0^{\Gamma_{ij}}$$
$$+ \frac{1}{N}\sum_{\mu=1}^{N_h}\sum_{\mathbf{k}'}{}' [\varepsilon(\mathbf{k}' + \mathbf{P}_\Gamma - \mathbf{Q}) - \varepsilon(\mathbf{k}')]\phi_i^\Gamma(\mathbf{p}_\mu, \mathbf{k}') , \tag{4a}$$

$$[\omega(\mathbf{Q}) - \varepsilon(\mathbf{k}) + \varepsilon(\mathbf{p}_\alpha)]\phi_i^\Gamma(\mathbf{p}_\alpha, \mathbf{k}) = \frac{1}{N}[\varepsilon(\mathbf{k} + \mathbf{P}_\Gamma - \mathbf{Q}) - \varepsilon(\mathbf{p}_\alpha)]\phi_0^\Gamma + \frac{1}{N}\sum_{\mathbf{k}'}{}' [\varepsilon(\mathbf{k}' + \mathbf{k} + \mathbf{P}_\Gamma - \mathbf{p}_\alpha - \mathbf{Q}) - \varepsilon(\mathbf{k}')]\phi_i^\Gamma(\mathbf{p}_\alpha, \mathbf{k}') , \tag{4b}$$

$$[\omega(\mathbf{Q}) - \varepsilon(\mathbf{k}) + \varepsilon(\mathbf{p}_i)]\phi_i^\Gamma(\mathbf{p}_i, \mathbf{k}) = \frac{1}{N}\sum_j [\varepsilon(\mathbf{k} + \mathbf{P}_\Gamma + \mathbf{p}_j - \mathbf{p}_i - \mathbf{Q}) - \varepsilon(\mathbf{p}_i)](-1)^{l_{ij}}\phi_0^{\Gamma_{ij}}$$
$$+ \frac{1}{N}\sum_{\mathbf{k}'}{}' [\varepsilon(\mathbf{k}' + \mathbf{k} + \mathbf{P}_\Gamma - \mathbf{p}_i - \mathbf{Q}) - \varepsilon(\mathbf{k}')]\phi_i^\Gamma(\mathbf{p}_i, \mathbf{k}') . \tag{4c}$$

Here the possible values of j are $j = i$ and the unfilled hole states in the partially filled shell of state Γ, l_{ij} is the number of occupied hole states in state Γ which lie in between states i and j, Γ_{ij} is the state obtained from Γ by removing the hole from state i and putting it in state j, and $\mathbf{P}_\Gamma$ is the total momentum of state Γ. The prime on the sum over $\mathbf{k}'$ indicates that the wave vectors of the filled shells and the partially filled shell are to be omitted.

Following Nagaoka[9] we find that if the $\{\mathbf{p}_\mu\}$ are all small, and also if $\mathbf{Q}$ is not very close to one or more of the wave vectors of the partially filled shell, then we can replace the $\{\mathbf{p}_i\}$ in Eq. (4) by zero. Also, if the energy $\omega(\mathbf{Q})$ is much less than the splitting between successive single-particle levels, which is of order $1/L^2$, then we can also replace $\omega(\mathbf{Q})$ in Eq. (4b) by zero in computing the *lowest-energy* solution, to which we confine our attention from now on. We then find that the lowest excitation energy can be expressed in terms of the result for one hole $\omega_1(\mathbf{Q})$ where

$$\omega_1(\mathbf{Q}) = \frac{4\pi}{N \ln N}\left[1 + O\left(\frac{1}{\ln N}\right)\right] , \tag{5}$$

in 2D, for $Q^2 \gg 1/\ln N$, *independent* of $\mathbf{Q}$ for $N \to \infty$, while in the opposite limit, $Q^2 \ll 1/\ln N$, one obtains a Q^2 spin-wave dispersion, i.e.,

$$\omega_1(\mathbf{Q}) = \frac{1}{N}\left(1 - \frac{2J^s}{1 + J^s}\right)Q^2 , \tag{6}$$

where, in $d = 2$,

$$J^s \equiv \frac{1}{N}\sum_{\mathbf{k}}{}' \frac{\sin^2 k_x}{2 - \cos k_x - \cos k_y} = 1 - \frac{2}{\pi} , \tag{7}$$

and the last equality in Eq. (7) is valid for $N \to \infty$. The logarithm of N appears in Eq. (5) because of the logarithmic divergence of the 2D sum $N^{-1}\sum'(2 - \cos k_x - \cos k_y)^{-1}$. In 3D one has[9] $\omega_1(\mathbf{Q}) = N^{-1}f(\mathbf{Q})$ where $f(\mathbf{Q})$ is a function of $\mathbf{Q}$, which can be evaluated in terms of various *finite* integrals. At long wavelengths this expression reduces to Eq. (6) with the corresponding 3D expression for J^s. We then find that the lowest excitation energies for the case of more than one hole are then given, in any dimension, by the eigenvalues of a matrix, $H^{\Gamma\Gamma'}$, whose size is the degeneracy of the Nagaoka state and whose elements are

$$H^{\Gamma\Gamma} = N_h\omega_1(\mathbf{Q}) , \tag{8a}$$

$$H^{\Gamma\Gamma'} = \begin{cases} (-1)^{l_{ij}}\omega_1(\mathbf{Q}) , \\ 0 , \end{cases} \tag{8b}$$

where the nonzero result in Eq. (8b) is for states $\Gamma \neq \Gamma'$ that are connected by transferring a single hole from state i to j. If Γ and Γ' are not connected by the transfer of a single hole, then the matrix element is zero. The matrix for two holes in 2D, for example, is of dimension 4, and has eigenvalues $(1,1,1,5) \times \omega_1(\mathbf{Q})$. From the structure of the matrix we find that, in general, the energy of the lowest branch is only determined by the number of holes

in *filled* shells, i.e.,

$$\omega(\mathbf{Q}) = N_f \omega_1(\mathbf{Q}) , \tag{9}$$

which is valid in any dimension. When there is no degeneracy, we see that the energy is just proportional to N_h, as found by Nagaoka,[9] but is otherwise somewhat less than this.

Note that the condition for the validity of our approximations is $N_h \ll \ln N$ in 2D. For larger values of N_h the spin-wave branch is no longer the excitation of lowest energy but is rather a resonance in a band of particle-hole excitations.[11] In three dimensions the approximations are valid for $N_h \ll N^{1/3}$. It is also straightforward to show that Eq. (9) also holds when one imposes more general boundary conditions on the single-particle wave functions.

When $\mathbf{Q}$ is very small, or more precisely when $\mathbf{Q}$ is very close to one of the wave vectors, $\{\mathbf{p}_i\}$, of the partially filled shell, we cannot entirely neglect the $\mathbf{p}$ dependence in Eq. (4). In this limit we find that the nonzero elements of $H^{\Gamma,\Gamma'}$ are

$$H^{\Gamma\Gamma} = \frac{1}{N}\left[N_h(\mathbf{Q}-\mathbf{P}_\Gamma)^2\left(1-\frac{2J^s}{1+J^s}\right)-2\mathbf{P}_\Gamma(\mathbf{Q}-\mathbf{P}_\Gamma)\right], \tag{10a}$$

$$H^{\Gamma\Gamma'} = \frac{(-1)^{l_{ij}}}{N}\left[(\mathbf{Q}-\mathbf{P}_\Gamma)(\mathbf{Q}-\mathbf{P}_{\Gamma'})\left(1-\frac{2J^s}{1+J^s}\right) - (\mathbf{p}_i+\mathbf{p}_j)\left(\mathbf{Q}-\frac{\mathbf{P}_\Gamma+\mathbf{P}_{\Gamma'}}{2}\right)\right], \tag{10b}$$

which reduces to Eqs. (6) and (8) when the $\mathbf{p}$ factors are neglected. Equation (10) is valid in any dimension provided that J^s is taken to be the appropriate d-dimensional integral.

In order to compare with numerical results on finite clusters it is necessary to understand the form of the *corrections* to the asymptotic form in Eqs. (5)–(10). To do so, we need to include corrections which come from excitations of more than one hole out of the Nagaoka state, for which we have developed a perturbation theory approach.[10] In 2D we find that the lowest excitation energy is given, for $Q^2 \gg 1/\ln N$, by

$$\omega(\mathbf{Q}) = \frac{1}{N}\left\{\frac{4\pi N_f}{\ln N}\left(1+\frac{a}{\ln N}+\cdots\right) + \frac{b}{N}\left[1+O\left(\frac{1}{\ln N}\right)\right]+\cdots\right\}, \tag{11}$$

where the coefficients a and b are both functions of $\mathbf{Q}$, so that degeneracy with respect to $\mathbf{Q}$ is lifted at subleading order, as well as of N_h. The coefficient b, which gives the leading contribution from the unfilled shell, is formally negligible in an expansion of powers of $1/\ln N$, but the coefficient is large, as we shall see, and so this term does give a significant contribution to the numerical results for the sizes that can be studied. States where two holes are excited from the Nagaoka state do not contribute to the leading term or to b. This justifies the neglect of such terms in the leading order results presented in Eqs. (5)–(10) above. In 3D, the leading-order correction is $N^{-1/3}$ rather than $1/\ln N$.

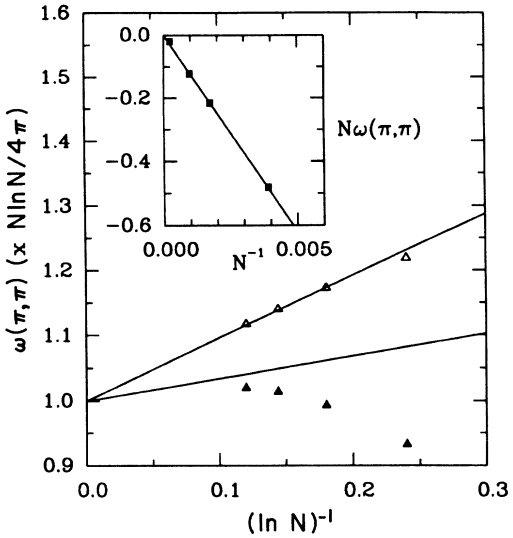

FIG. 1. Plot of $\omega(\pi,\pi)(\times N\ln N/4\pi)$ for one hole in 2D both with periodic boundary conditions (open triangles) and with boundary conditions which shift the single-particle wave vectors by $2\pi L^{-1}(\frac{1}{4},\frac{1}{4})$ (filled triangles). The sizes are between $L=8$ and $L=64$. The straight lines show the analytic predictions valid for large N, i.e., $\omega(\pi,\pi)(\times N\ln N/4\pi)=1+a/\ln N$ where $a=0.9594$) for periodic boundary conditions and $a=0.3407$ for the shifted boundary conditions. The agreement is seen to be good, particularly for periodic boundary conditions. The inset shows $N\omega(\pi,\pi)$ plotted against N^{-1} for antiperiodic boundary conditions, for which the Nagaoka state is fourfold degenerate and $N_f=0$. The sizes are between $L=16$ and $L=64$. The results agree very well with the analytic result $\omega=-4\pi^3/N^2$, shown by the solid line.

In order to verify our predictions we have also directly diagonalized the eigenvalue problem in Eq. (2), using the Lanczos algorithm.[12] Figure 1 shows results obtained for $\omega(\pi,\pi)(\times N\ln N/4\pi)$ plotted against $1/\ln N$ for 1 hole, both for periodic boundary conditions and for boundary conditions in which the single-particle wave vectors are shifted by $2\pi/L(\frac{1}{4},\frac{1}{4})$. From Eq. (11), it follows that this should equal N_f ($=1$ here), in the thermodynamic limit, with a slope equal to a neglecting the b/N and higher-order terms in Eq. (11). We find that $a=0.9594$ for periodic boundary conditions and $a=0.3407$ for the shifted boundary conditions. As seen in Fig. 1, the numerical results agree with these predictions, though higher-order corrections seem larger for the shifted boundary conditions. We have also computed $\omega(\pi,\pi)$ for antiperiodic boundary conditions, i.e., the wave vectors are shifted by $2\pi/L(\frac{1}{2},\frac{1}{2})$, for which the Nagaoka state is four-fold degenerate, and $N_f=0$, so the leading term in Eq. (11) is b/N^2. A calculation gives $b=-4\pi^3$, which agrees well with our numerical results, as shown in the inset to Fig. 1.

In Fig. 2 we show results for two holes for a range of sizes up to $L=24$. From Eq. (11) the asymptotic value is predicted to be 1, which seems to be consistent with the results. Note the change of sign, indicated by the points crossing the line as discussed in the caption, which occurs for intermediate sizes. Fang *et al.*[6] found an instability at $\mathbf{Q}=(\pi,0)$ for sizes up to $L=10$. While we agree with

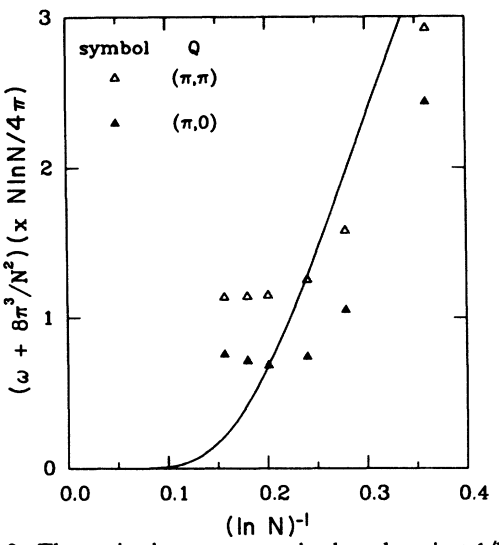

FIG. 2. The excitation energy, ω, is plotted against $1/\ln N$ for two holes for $\mathbf{Q}=(\pi,\pi)$ and $(\pi,0)$. The sizes are between $L=4$ and $L=24$. We have subtracted from ω the b/N^2 term in Eq. (11), where we find $b=-8\pi^3$. Although this term would be negligible for sufficiently large N compared with the logarithmic corrections in Eq. (11), the coefficient is very large so that it does make a large contribution for the sizes studied. We have also multiplied by $N\ln N/4\pi$, so the asymptotic value should be 1, i.e., N_f rather than N_h, and the data appears to be consistent with this. The solid line is the result obtained if the frequency were $8\pi^3/N^2$. Hence the actual frequency is given by the difference between the points and the solid line, which changes from negative to positive for $L\gtrsim 12$ for $\mathbf{Q}=(\pi,0)$ and $L\gtrsim 8$ for $\mathbf{Q}=(\pi,\pi)$.

their results for the sizes that they studied, we see that this mode, in fact, becomes *stable* at larger sizes. However, we do find unstable modes for two holes at *small* $\mathbf{Q}$ for two holes. Results obtained from the reduced Hamiltonian in Eq. (10) are presented in Table I, along with the results of directly diagonalizing the original Hamiltonian for finite sizes. We see that the agreement between the two sets of results is quite good. In all cases the *sign* of the energy is given correctly for the largest size. Presumably this long wavelength instability is the one reported by Doucot and Wen.[7] In addition to $N_h=2$ we find a small number of unstable long wavelength modes for $N_h=2$–4, 7, 15–19 in two dimensions. However, for larger hole numbers (we have checked explicitly up to $N_h=37$) we do not find any unstable modes, even at long wavelengths, because of the factor of N_h with a positive coefficient on the

TABLE I. Results for $[N/(2\pi)]^2\omega(\mathbf{Q})$ for two holes in two dimensions with periodic boundary conditions, where $\mathbf{Q}=2\pi L^{-1}(n_x,n_y)$. In these units the value for one hole is $n_x^2+n_y^2$. The results marked $N=\infty$ are obtained from Eq. (10) of the text while the results for finite N are obtained by diagonalizing the Hamiltonian, given by Eq. (2). The eigenvalue on the second row is 0 because $\mathbf{Q}=(0,1)$ is the wave vector of the Nagaoka state, so we just obtain the rotated state of the same energy with S^z reduced by one. Note that only a finite number of long wavelength modes are unstable. Note that the energies increase with increasing system size. For $L=\infty$ our calculations predict that the energy is positive for *all* other $\mathbf{Q}$ values and the numerical results appear to confirm this, though we have not checked all possible $\mathbf{Q}$ values for $L=24$.

(n_x,n_y)	$L=\infty$	$L=16$	$L=24$
(0,0)	0.467	0.269	0.378
(0,1)	0	0	0
(0,2)	−1.324	−1.449	−1.384
(0,3)	−0.965	−1.424	−1.196
(0,4)	0.853	−0.354	0.219
(1,1)	−0.477	−0.472	−0.477
(1,2)	−1.159	−1.284	−1.227
(1,3)	−0.580	−1.087	−0.848
(1,4)	1.324	0.003	0.611
(2,2)	−0.643	−0.909	−0.804
(2,3)	0.544	−0.204	0.108
(3,3)	2.369	0.980	1.511

diagonal of $H^{\Gamma\Gamma'}$ in Eq. (10). We have been unable to find *all* the values of N_h in 3D for which there is a long wavelength instability because the degeneracy of the matrix in Eq. (10) becomes too great. We were able to check that the instability does occur for $N_h=2$–5, 10, 11, 15. However, it is clear that, just as in 2D, the instability will not persist for large N_h.

To conclude, we have demonstrated that the instability found in earlier calculations[5–8] is an artifact of the small sizes and the particular hole numbers used. The saturated ferromagnetic state is generically *locally stable* with respect to flipping a single spin for $N_h \ll \ln N$, in two dimensions ($N_h \ll N^{1/3}$ in three dimensions).

It is a pleasure to thank David Edwards for most helpful suggestions and correspondence. We are also grateful to Josh Deutsch and Sriram Shastry for many helpful discussions. This work was supported in part by National Science Foundation Grant No. DMR 87-21673. J.A.R. was financially supported by the Consejo Nacional de Investigaciones Científicas y Técnicas de la Argentina.

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