Instability of the Nagaoka ferromagnetic state of the $U=\infty$ Hubbard model

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We identify a "k_F instability" of the Nagaoka ferromagnetic state of the $U=\infty$ Hubbard model. We show rigorously that for a large enough hole concentration the ferromagnet possesses an instability with respect to overturning an up-spin electron at the Fermi surface and placing it at the bottom of a down-spin band made very narrow by correlation effects. We find a low-energy scale for spin waves in this strong-coupling limit, in the form of a spin-wave stiffness that is much smaller than its random-phase-approximation value.

In this paper we present some variational and exact results concerning the Hubbard model in the limit of large U—pertaining mainly to the stability or otherwise of the Nagaoka ferromagnet. The result of Nagaoka[1] (see also Thouless[2]) is of considerable importance since it is a nonperturbative and exact statement about the Hubbard model for strong coupling, i.e., $U=\infty$. The recent revival of interest in the Hubbard model for large (but not infinite) U, following Anderson's suggestion[3] of its relevance in high-T_c superconductivity, has focused mainly on the so-called Heisenberg-Hubbard model, which in fact contains the $U=\infty$ Hubbard model kinetic energy as one of its two pieces. In addition, the theory of itinerant electron ferromagnetism has traditionally relied upon the Nagaoka ferromagnet as a clearly demonstrable case of the existence of ferromagnetism in a one-band Hubbard model.[4]

Given the importance of the Nagaoka ferromagnet, the "thermodynamic frailty" of the methods used to prove it have been a source of concern to several workers over the years. Nagaoka shows that the fully saturated ferromagnet is a ground state in the case of one hole (measured from half-filling) for $U=\infty$ and on appropriate lattices. This method fails to prove ferromagnetism for a few as two holes. In fact in the case of two holes we can readily show, by essentially a Peierls construction, that a singlet state must exist with an energy only $O(1/L^2)$ above that of the ferromagnet (we could cut the lattice into two equal domains and confine one hole into each, and further form the largest spin state for each domain and couple these two domain ferromagnets into a singlet—the energy cost is only a boundary effect). For a thermodynamic concentration of holes, such considerations really do not serve as proper guides. However, the one-dimensional Hubbard model, with $U=\infty$, has a separation of charge and spin, and so it is impossible to find a state with lower energy than the Nagaoka state at any concentration of holes. This leads to a possible scenario in which the ferromagnet could survive (at $U=\infty$) in two and three dimensions for *any* hole concentration.

It is the purpose of this paper to show that the preceding scenario is false—we present a variational wave function with one spin down with a finite wave vector, k_F, which has a lower energy than the Nagaoka state in two and three dimensions for a sufficiently large concentration of holes. Our "excitation energy" is a strict upper bound to the true excitation energy, and becomes negative for large enough δ (density of holes) but it remains non-negative in one dimension. In fact, our criterion for the instability of the ferromagnet (namely the "excitation energy" going negative) captures the subtleties of the Nagaoka theorem (related to the signs of the hopping matrix element on nonbipartite lattices). We also present variational estimates on how large the Coulomb interaction U must be in order to stabilize the ferromagnet. These are, however, not optimal for all δ. We believe that this is the first published demonstration of the instability of the Nagaoka state for any hole concentration (at $U=\infty$) which has a variational (and hence rigorous) basis, and which is thermodynamically relevant.

In order to motivate our wave functions, we would like to review, briefly, the work of Richmond and Rickayzen,[5] who performed an interesting calculation with a similar objective to ours. These authors also consider the problem of $N_\uparrow=N_s(1-\delta)$ up (-spin) electrons and one down (-spin) electron N_s being the number of lattice sites) and construct a variational wave function obtained by freezing the motion of the down electron and solving exactly for the up electron gas which now sees a simple potential scatterer (strength U) at one site. The up-electron energies are shifted by $O(1/N_s)$ each, and the net cost is $O(1)$, whereas the possibility of virtually admixing the doubly occupied site gains an exchange energy. The final conclusion of this study is that the Nagaoka ferromagnet is unstable with respect to reducing U from infinity—however, they find that at $U=\infty$ the Nagaoka ferromagnet is always stable for any δ.

It appears that the preceding stability of the Nagaoka ferromagnet arises in their calculation by the inability of the wave function to allow the down-spin electron to hop around. The overturned electron would prefer to be in a highly delocalized state. For, if we imagine the fully spin-polarized Stoner state (which is just the Nagaoka state at $U=\infty$) and switch off U, then the leading instability would correspond to destroying an up electron at the (Stoner-Nagaoka) Fermi surface and creating a down electron at the band bottom. This picture immediately suggests that an appropriate strategy for the large-U problem would be to take such a "Fermi surface restoring" excitation and to correct for strong Coulomb repulsion by a variational projection.

Explicitly we write the Hamiltonian

$$H=-\sum_{ij} t_{ij} C_{i\sigma}^{\dagger} C_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \ . \tag{1}$$

In the $U=\infty$ limit, the above considerations lead us to the variational wave function[6]

$$|\chi_v\rangle = (N_s)^{-1/2} \sum_m e^{iqr_m} C_{m\downarrow}^{\dagger}(1-n_{m\uparrow}) C_{k_F\uparrow} |F\rangle \ , \tag{2}$$

where $|F\rangle$ is the ferromagnetic Nagaoka-Stoner state $\prod_{0\le|k|\le k_F} C_{k\uparrow}^{\dagger}|\text{vac}\rangle$, and k_F refers to one of the Fermi surface vectors. A straightforward calculation gives the excitation energy

$$\langle \chi_v|(H-E_0)|\chi_v\rangle / \langle \chi_v|\chi_v\rangle \ ,$$

where E_0 is the energy of the Nagaoka-Stoner state, as

$$\lambda_v(q) = (\hat{\mu}-\varepsilon_F) + \varepsilon_q \delta (1-\hat{\mu}^2/z^2t^2) \ . \tag{3}$$

Here $\rho \equiv 1-\delta$, $\hat{\mu} \equiv -E_0/(N\delta)$, and $\varepsilon_F \equiv \varepsilon_{k_F}$, with

$$\varepsilon_k = -(1/N_s) \sum_{ij} t_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} \ ,$$

z = coordination number and further we assume that $t_{ij}=t$ for i,j nearest neighbor and zero otherwise. In terms of the density of states $\rho(\varepsilon)$ per site and per spin we have

$$\hat{\mu}\delta = \int_{\varepsilon_F}^{W_{\text{top}}} \varepsilon \rho(\varepsilon) d\varepsilon \quad \text{and} \quad \delta = \int_{\varepsilon_F}^{W_{\text{top}}} \rho(\varepsilon) d\varepsilon \ , \tag{4}$$

where W_{top} is the band top energy, whence $\varepsilon_F \le \hat{\mu} \le W_{\text{top}}$. In Eq. (3), the two terms are, respectively, the energy loss of the up spins brought about by the up electrons having to avoid the inserted down spin (it is a net loss since $\hat{\mu} \ge \varepsilon_F$) and the energy gain of the down electron that can move around on the vacant sites left behind in the ferromagnet. The coefficient of ε_q in (3) represents the effective "band width" reduction factor of the down electron—which is, in fact, the hole-density–hole-density correlation function at nearest-neighbor separation in the Nagaoka ferromagnet divided by δ. The physics of this term is simply that given a hole at a site, a down spin is inserted there, and its hopping requires a hole at a neighboring site—thus we need the conditional probability of finding a second hole at a nearest-neighbor site given one hole at a site.

Clearly the lowest value of $\lambda_v(q)$ is obtained by setting ε_q as the band bottom energy $-|W_{\text{bot}}|$. We distinguish two cases here depending on whether (a) $W_{\text{top}}=z|t|$ or (b) $W_{\text{top}}<z|t|$. Case (a) applies to the square lattice, the triangular lattice with $t<0$, the simple cubic, the bcc lattice, and the fcc lattice with $t<0$. Case (b) corresponds to the triangular and fcc lattices with $t>0$. We assert for all the lattices in case (b) that the ferromagnet is unstable for arbitrarily small δ; the instability is of course exactly what Nagaoka's theorem would predict for a single hole— it arises in (3) because the first term is a positive number of $O(\delta)$ and the second is also of $O(\delta)$ but negative, with a larger coefficient. Case (a) is, however, more subtle. The fact that $W_{\text{top}}=z|t|$ and Eq. (4) imply that $(\hat{\mu}/zt)^2$ tends to 1 as $\delta\to 0$, whence the second term in (3) is of $O(\delta^2)$. This guarantees that there must exist a nonzero region around $\delta=0$ where λ_v is non-negative—this robustness of the Nagaoka ferromagnet in this case stems from the rather curious fact that the hole-density–hole-density correlation function of the ferromagnet, at nearest-neighbor separation, is of $O(\delta^3)$ rather than $O(\delta^2)$ as one might naively expect. In effect holes repel very strongly in this case thereby enhancing the stability of the Nagaoka state. Table I lists the critical values of δ above which λ_v goes negative in various cases. It is seen that there are surprisingly stable cases—the case (a) triangular lattice and fcc lattice, which appear to be good candidates for itinerant ferromagnetism.

Having found an excitation with possibly vanishing energy, we observe that the preceding instability has a wave vector corresponding to the Stoner-Nagaoka Fermi momentum relative to the band bottom state's momentum. This is a generalized spin wave with a (fixed) nonzero wave vector $q=k_F$; and brings us to the question of the (Goldstone) long-wavelength spin waves, which must on symmetry grounds possess a vanishing energy.[7] We therefore construct a variational wave function which contains long-wavelength spin waves and also interpolates to contain the leading instability already discussed as

$$|\phi\rangle = \frac{1}{\sqrt{\beta(N_s-N)}} \sum_{m,k} e^{i(k+q)r_m} \psi_k C_{m\downarrow}^{\dagger}(1-n_{m\uparrow}) C_{k\uparrow}|F\rangle, \tag{5}$$

where ψ_k is an unspecified amplitude for the wave vector k. The wave function[8] $|\phi\rangle$ is characterized by the wave vector q, and is motivated by the RPA (Ref. 9) which can be recovered by neglecting the (projection) factor $(1-n_{m\uparrow})$. If we choose ψ_k to be a Kronecker δ function at $k=k_F$, this reduces to our wave function $|\chi_v\rangle$ in Eq. (2). If we set $q=0$ and let ψ_k be independent of k, then $|\phi\rangle$ is simply the state obtained by acting on $|F\rangle$ with the total spin lowering operator, and hence is degenerate with $|F\rangle$.

The constant β in (5) is determined by normalization as

$$\beta = \sum_k |\psi_k|^2 f_k + \frac{1}{N_s\delta} \sum_{p,k} \psi_p^* \psi_k f_p f_k \ , \tag{6}$$

where $f_k = \Theta(\varepsilon_F-\varepsilon_k)$ restricts the sum to the Stoner-Nagaoka Fermi sea. We calculate the "spin-wave" excitation energy [i.e., $\langle\phi|(H-E_0)|\phi\rangle$] to be

TABLE I. The spin-wave stiffness in our scheme and in the RPA, in units of zt where z is the coordination number for different lattices, and the critical hole concentration δ_{cr} where Eq. (3) is zero.

		Square	Triangle	sc	bcc	fcc
$\delta=0.1$	D_{RPA}	0.023	0.03	0.012	0.01	0.006
	D	0.009	0.016	0.006	0.005	0.004
$\delta=0.2$	D_{RPA}	0.044	0.056	0.024	0.015	0.01
	D	0.014	0.026	0.007	0.006	0.006
δ_{cr}		0.49	1	0.32	0.32	0.62

$$\varepsilon(q)=\frac{1}{\beta}\sum_k \lambda_k(q)\psi_k^*\psi_k f_k + \frac{1}{\beta N_s}\sum_{kp} f_k f_p \psi_p^*\psi_k K(k,p;q) , \tag{7}$$

where

$$\lambda_k(q)=\hat{\mu}-\varepsilon_k+\delta(1-\hat{\mu}^2/z^2t^2)\varepsilon_{k+q} \tag{8}$$

and

$$K(k,p;q)\equiv(\varepsilon_{k+q}+\varepsilon_{p+q})+(\hat{\mu}/zt)(\varepsilon_q+\varepsilon_{k+p+q}) . \tag{9}$$

Varying with respect to ψ_k^*, with the preceding normalization constraint, we find the eigenvalue equation

$$[\varepsilon(q)-\lambda_k(q)]\psi_k=\frac{1}{N_s}\sum_p f_p \left[K(k,p;q)-\frac{1}{\delta}\varepsilon(q)\right]\psi_p . \tag{10}$$

This integral equation has two classes of solutions, the continuum of scattering states obtained by omitting the right-hand side [which shifts the energies only by $O(1/N)$] and a bound state, the (Goldstone) spin wave, starting at zero energy at $q=0$. The scattering continuum is analogous to the Stoner particle-hole continuum in the weak-coupling ferromagnet, and is bounded from below by the minimum of $\lambda_k(q)$ for a given q. Its value at $q=0$ is the effective exchange splitting in this strong-coupling theory. The instability discussed in the previous sections is precisely contained in this scheme, since $\lambda_k(q)$ at $\mathbf{q}=\mathbf{k}_f$ has a minimum at $\mathbf{k}=-\mathbf{k}_F$, thus our previous discussion is tantamount to the statement that the lower edge of the scattering continuum has a minimum at $q=k_F$, and that this minimum comes down with increasing δ, until at some critical value, it hits the abscissa, signifying the instability of the ferromagnet.[10] This scheme also contains the Goldstone mode, since a calculation shows that Eq. (7), in the limit of $q=0$, has a zero eigenvalue with the eigenfunction ψ_k independent of k. (This phenomenon is a statement of the rotational invariance of our scheme.)

The small-q spin-wave spectrum can be extracted from the (separable kernel) integral equation (10). We find the eigenfunction

$$\psi_k=1+q_x\phi_k+O(q_x^2) ,$$

and ϕ_k is obtained as

$$\phi_k=\frac{v_{k_x}}{\lambda_k(0)}\frac{1}{1+z\hat{\mu}I/(2\theta)} , \tag{11}$$

where

$$v_{k_x}=(\partial/\partial k_x)\varepsilon_k ,$$

and

$$I=(1/N_s)\sum_k f_k v_{k_x}^2/\lambda_k(0) .$$

These are appropriate in all the lattices of case (a), with energy measured in units of W_{top}. In the remainder of the paper, we use the same units. The constant $\Theta=1$ in all cases except the triangular lattice where $\Theta=2$, and we treat this lattice as a square lattice (with lattice constant a) and all diagonal bonds running, say, northeast. The spin-wave energy goes as

$$\varepsilon_{SW}(q)=Dq_x^2a^2+O(q^4) ,$$

with the stiffness given (in units of zt) by

$$D=D_{RPA}\left[1-\frac{Iz}{\hat{\mu}\Theta(1+\hat{\mu}Iz/2\Theta)}\right] , \tag{12}$$

where $D_{RPA}=\Theta\hat{\mu}\delta/z$. Note that I is always positive, and hence the spin waves are always softer than what RPA suggests. In Table I we list the stiffness for two typical values of δ (0.1 and 0.2) and also the RPA values for comparison.

It is remarkable that the stiffness is much smaller than D_{RPA}, and 2 orders of magnitude less than zt is almost all the cases considered. This low-energy scale of the long-wavelength excitations would lead to a transition temperature that is considerably lower than the Stoner-Hartree-Fock estimates, and has a bearing on the question of why the T_c of itinerant ferromagnets is so low[11] (spin-wave theory[12] for the simple cubic lattice for $\delta=0.2$ would give a $T_c=0.029\ z|t|$). In any case our calculation gives an upper bound on the spin-wave stiffness. A finite exchange energy (t^2/U) would reduce this further.

For general nonzero q, the integral equation (10) reduces to a set of algebraic equations by using the separability of the kernel, and was solved numerically. In Fig. 1 we sketch the bound-state spectrum and the scattering continuum for the square lattice in two cases; one case

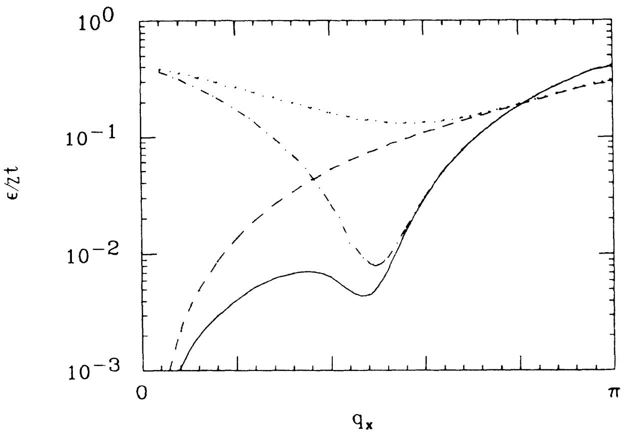

FIG. 1. The spin-wave energy (solid and dashed curves) and the bottom of the scattering continuum (dot-dashed and dotted curves) for $\delta \lesssim \delta_{cr}$ and $\delta \sim 0.34$, respectively, on a logarithmic scale, against q [along (1,1) direction].

corresponds to a small enough δ for which we only have positive-definite excitations, and the second corresponds to $\delta \sim 0.49$ at which the Nagaoka ferromagnet is close to being unstable.

From Fig. 1, it is seen that the spin-wave bound state is at a much lower scale than the single-particle continuum, and unlike in the usual weak-coupling case, does not enter the continuum for any q. The effect of increasing the hole density is to bring down the entire continuum rapidly, and the dip at $q = k_F$ precipitously. This situation is somewhat reminiscent of soft modes in ferroelectrics, but is a more severe instability since essentially an infinite number of states are going soft. The spin waves respond by going soft slightly before $q = k_F$, and hug the bottom of the continuum for larger q.

We have also used a simple generalization of the wave function of Eq. (2) to determine the critical value of U below which the Nagaoka state is definitely unstable. The variational function is chosen as a Gutzwiller incomplete projected version of Eq. (2) and written as

$$|\Phi_G\rangle = \prod_m [1+(g-1)n_{m\uparrow}n_{m\downarrow}]C^\dagger_{q\downarrow}C_{k_{F\uparrow}}|F\rangle , \qquad (13)$$

where g is the usual Gutzwiller parameter. The variational energy now reads

$$\lambda_v(g,q,U) = C^{-1}\{(g-1)^2\hat{\mu}\delta - C\varepsilon_F + g^2\rho U + \varepsilon_q[(\delta+\rho g)^2 - \delta^2(g-1)^2\hat{\mu}^2]\} , \qquad (14)$$

where $C = \delta + \rho g^2$, $\rho = 1-\delta$, and the various terms are recognizable in analogy with Eq. (3) (obtained by $g \to 0$), except the third which is the Coulomb interaction energy. For a fixed δ and U, we can minimize Eq. (14) with respect to g; and U_{cr} is defined by $\lambda_v = 0$. We believe that this estimate of U_{cr} is a reasonably good guide for $\delta \to \delta_{cr}$, where U_{cr} diverges [like $(\delta_{cr}-\delta)^{-1}$]; but is far from optimal for $\delta \to 0$. In the limit of small δ and large U, the main contribution to the excitation energy comes from the first, second, and last term [i.e., by ignoring the kinetic energy of the down spin which is of $O(\delta^2)$], and we find the leading behavior goes as $(\hat{\mu}-\varepsilon_F) - \delta\hat{\mu}^2/U$. Thus, both terms are of order δ and hence we find that in order to stabilize the ferromagnet we must have $U > U_1$ with U_1 an $O(1)$ energy $\{=\lim_{\delta\to 0}[\delta\hat{\mu}^2/(\hat{\mu}-\varepsilon_F)]\}$. This is not as good as the result of Richmond and Rickayzen, who find the exchange contribution [i.e., term of $O(t^2/U)$] to be independent of δ, whereby $U_{cr} \to \infty$ as $\delta \to 0$. Their result is of course more reliable in this limit since their calculation is exact whenever the down-electron kinetic energy is neglected. In Fig. 2, we juxtapose for the square lattice our result for the stability regime with that of Ref. 4 for the case of the square lattice, to get a rigorous limit on the regime of stability of the Nagaoka ferromagnet.

In summary, we have shown in this paper that the Nagaoka ferromagnet is unstable for a sufficiently large concentration of holes at $U = \infty$ by identifying a soft Fermi-surface restoring excitation. The Nagaoka-Stoner Fermi surface forces the kinetic energy of the up electron to be much greater than that in the Luttinger, or normal (Fermi liquid) Fermi surface, and the instability corresponds to the rectification of this state of affairs—for large enough δ, the down-electron band width becomes large enough to benefit from this collapse. Our estimate of the down-electron band width as $O(\delta^2)$, rather than $O(\delta)$ is specific to the use of our variational wave function—if this is true in general then we have a generic argument for the stability of the Nagaoka ferromagnet for small enough δ. If a state can be found that has a band width for down electrons of $O(\delta)$ while costing only an energy of $O(\delta)$ for the up spins, then it would be possible to destabilize the ferromagnet for any $\delta > 0$. Although we cannot rule out this possibility categorically, we feel it is unlikely since our wave function can only be improved upon by an admixture of particle-hole excitations in the up-electron Fermi surface, which should be quite small [to keep the up-electron energy cost low, of $O(\delta)$].

The instability, with respect to reducing U from

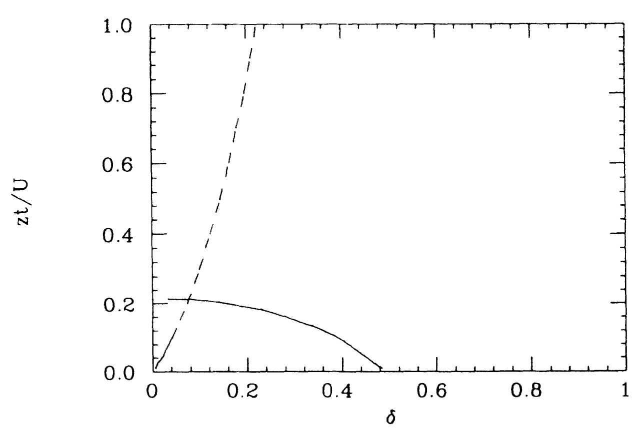

FIG. 2. zt/U_{cr} vs δ for the square lattice as found from our Eq. (14) (solid line) and from Ref. (4) (dashed line). The Nagaoka ferromagnetic is then definitely unstable outside the area bounded by the two curves and the abscissa.

infinity, occurs in two physically distinct ways. One is that at low δ the exchange energy of $O(t^2/U)$ competes with the ferromagnet and leads, presumably through a first-order transition, to an antiferromagnetically correlated state. In the other regime of $\delta \lesssim \delta_{cr}$, we find that terms of $O(1/U)$ bring down the strong coupling continuum to a lower energy, and the k_F instability becomes more pronounced—leading again, we suspect, via a first-order transition—to a metal with a normal Luttinger-like Fermi surface and strong antiferromagnetic correlations.

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[5]P. Richmond and G. Rickayzen, J. Phys. C **2**, 528 (1969).

[6]This wave function turns out to have a long history, and was first written down by Laura M. Roth, J. Phys. Chem. Solids **28**, 1549 (1967), who, however, seems to have missed the instability contained in it, which we discuss in what follows. The same wave function has also been rediscovered by S. Schmitt-Rink and A. Ruckenstein (unpublished).

[7]In the case of the electron gas the ferromagnetic state, found within the Hartree-Fock approximation by Bloch, was shown to be unstable with respect to long-wavelength spin-wave excitations in a small range of r_s by Herring [C. Herring, *Magnetism*, edited by G. T. Rado and H. Suhl (Academic, New York, 1966), Vol. IV, p. 104]. It is therefore necessary to examine the long-wavelength spin waves to make sure of the stability of the ferromagnet.

[8]This wave function has also been discussed by L. M. Roth (Ref. 5) who used it only to study the long-wavelength spin waves.

[9]Reviewed by C. Herring in Ref. 7, Chap. XIV. (By RPA we refer to the limit $U=\infty$ of the RPA results noted in this review).

[10]A similar instability of the Nagaoka-Stoner state has also been discussed by Laura M. Roth, Phys. Rev. **186**, 428 (1969), using a Green's-function decoupling scheme. Even though her considerations did not have a variational significance, B. W. Tan, in his unpublished thesis (Imperial College, London, 1974) has shown that Roth's decoupling scheme results can be obtained using a variational wave function for one-spin-down excitations. See also D. M. Edwards and J. A. Hertz, J. Phys. F **3**, 2191 (1973); S. R. Allan and D. M. Edwards, J. Phys. F **12**, 1203 (1982).

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[12]We are using a crude estimate taken from a simple minded spin-wave calculation, which gives $\Delta M/M(0)=(0.0587/S)(k_B T/D)^3/2$, [see, e.g., C. Kittel, in *Introduction to Solid State Physics*, Sixth Ed. (Wiley, New York, 1986), p. 435], and use $S=\frac{1}{2}$ with $\Delta M/M(0)=1$ in order to find the estimate quoted in the text.