# Metallic ferromagnetism in a single-band model. III. One-dimensional half-filled band

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A single-band model recently proposed to describe metallic ferromagnetism is studied in a one-dimensional geometry in the half-filled-band case. The model describes a tight-binding band with on-site repulsion $U$ and nearest-neighbor Coulomb exchange matrix element $J$. We determine the parameter regimes that give rise to partial and full spin polarization using exact diagonalization and analytic techniques. Ferromagnetism only occurs for $J \neq 0$, with the required value of $J$ decreasing as $U$ increases and approaching zero as $U \to \infty$. A regime of partial spin polarization is found to exist for $U$ less than the bandwidth. We examine the validity of mean-field theory for this model and find it to be remarkably effective in describing its physical properties.

## I. INTRODUCTION

The single-band Hamiltonian

$$H = -t \sum_{\substack{\langle ij \rangle \\ \sigma}} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + J \sum_{\substack{\langle j \rangle \\ \sigma\sigma'}} c_{i\sigma}^{\dagger} c_{j\sigma'}^{\dagger} c_{i\sigma'} c_{j\sigma} \tag{1}$$

has recently been proposed as a simple model containing the essential physics of metallic ferromagnetism.[1] The parameter $J$, that drives ferromagnetism in this model, is an off-diagonal matrix element of the Coulomb interaction between electrons in nearest-neighbor sites and is *positive*, and $U$ is the usual Hubbard on-site repulsion.

Within mean-field theory, the Hamiltonian Eq. (1) gives rise to ferromagnetism if the parameters $J$ and/or $U$ are large enough.[1] In particular, even for $J=0$ one obtains ferromagnetism for sufficiently large $U$ when the Stoner criterion[2]

$$Ug(\varepsilon_F) > 1 \tag{2}$$

is satisfied, where $g(\varepsilon_F)$ is the density of states at the Fermi energy. However, it is well known that mean-field theory overestimates the effect of $U$ by not taking into account the ability of electrons of opposite spin to avoid each other (correlations). In fact, it is likely that the Hamiltonian Eq. (1) never exhibits ferromagnetism if $J=0$.[3] On the other hand, it is intuitively obvious that ferromagnetism in this model will occur for sufficiently large $J$. Thus, it was conjectured in Ref. 1 that mean-field theory may not be unreasonable as far as the treatment of the interaction $J$ is concerned, and that the effect of correlations may be taken into account in the mean-field equations by using an "effective" value of $U$ which is smaller than the bare $U$ and does not satisfy the Stoner criterion. Our results in this paper support this conjecture.

We study in this paper the parameter range giving rise to ferromagnetism in the model Eq. (1) for the special case of a one-dimensional lattice.[4] In addition, we restrict ourselves to the half-filled-band case. The condition on the parameters to give rise to full spin polarization can be found exactly, as shown in Sec. II, and is found to coincide with the prediction of mean-field theory for small $U$. The value of $J$ required for ferromagnetism decreases monotonically with $U$ and approaches zero for large $U$, but always remains finite. The mean-field solution for this model, also discussed in Sec. II, exhibits certain differences from the case of constant density of states discussed in Ref. 1. In particular, it exhibits a finite jump in the magnetization for certain parameters, in agreement with the exact solution. In Sec. III we study the condition for onset of partial spin polarization by exact diagonalization of small lattices. A regime of partial spin polarization is found to exist only for $U$ less than the bandwidth, in qualitative agreement with mean-field predictions. We conclude in Sec. IV with a summary of results and a discussion of the validity of mean-field theory.

## II. ANALYTIC RESULTS

The Hamiltonian Eq. (1) can be rewritten as

$$H = -t \sum_{i\sigma} (c_{i\sigma}^{\dagger} c_{1+1\sigma} + \text{H.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \frac{J}{2} \sum_{\langle ij \rangle} (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + n_i n_j) \tag{3}$$

which makes its rotational invariance apparent. We have also specialized to the one-dimensional case. Let us consider first the simple limiting case $U \to \infty$. The usual transformation applies, and Eq. (3) becomes

$$H_{\text{eff}} = \left( \frac{t^2}{U} - \frac{J}{2} \right) \sum_{\langle ij \rangle} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \equiv J_{\text{eff}} \sum_{\langle ij \rangle} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \ . \tag{4}$$

We have dropped the term in Eq. (3) involving $n_i n_j$ as it is irrelevant in the large-$U$ limit for the half-filled case. The Heisenberg Hamiltonian Eq. (4) has ferromagnetic long-range order for $J_{\text{eff}} < 0$ and a singlet ground state with "almost" antiferromagnetic long-range order for $J_{\text{eff}} > 0$. Thus, the condition for ferromagnetism in this limit is $J_{\text{eff}} < 0$, or

 

$$J > J_c = \frac{2t^2}{U} \ . \tag{5}$$

Note that this condition remains the same for a higher-dimensional hypercubic lattice. In that case, the ground state has true antiferromagnetic long-range order for $J < J_c$.

We next consider the predictions of mean-field theory. A mean-field decoupling of the interactions in the Hamiltonian Eq. (3) leads to the Hamiltonian

$$H_{\rm mf} = \sum_{k\sigma} E_\sigma(k) c_{k\sigma}^\dagger c_{k\sigma} \tag{6}$$

with

$$E_\sigma(k) = -2(t - JI_1)\cos k - \sigma\frac{U+2J}{2}m \ , \tag{7}$$

$$I_1 = \tfrac{1}{2}\sum_\sigma \langle c_{i\sigma}^\dagger c_{i+1\sigma} + \text{H.c.}\rangle \ , \tag{8}$$

and

$$m = n_\uparrow - n_\downarrow \tag{9}$$

the magnetization per site. The condition on the parameters to yield spin polarization is obtained by setting

$$E_\uparrow(k_{F\uparrow}) = E_\downarrow(k_{F\downarrow}) \tag{10}$$

with $k_{F\uparrow}, k_{F\downarrow}$ the Fermi wave vectors for up and down electrons, given by

$$k_{F\uparrow} = \frac{n+m}{2}\pi \ , \tag{11a}$$

$$k_{F\downarrow} = \frac{n-m}{2}\pi \ . \tag{11b}$$

Equation (10) then yields

$$4t\sin\frac{n\pi}{2}\sin\frac{m}{2}\pi\left[1 - \frac{J}{t}I_1\right] = (U+2J)m \tag{12}$$

and $I_1$ is obtained from

$$I_1 = \frac{2}{N}\sum_k \cos k\,(n_{k\uparrow} + n_{k\downarrow}) \tag{13}$$

as

$$I_1 = \frac{2}{\pi}\sin\frac{n\pi}{2}\cos\frac{m\pi}{2} \ . \tag{14}$$

The condition on $J$ to obtain a given magnetization $m$ is then

$$J = 2tc\frac{1-(U/4tc)[m/\sin(m\pi/2)]}{[m/\sin(m\pi/2)] + (4/\pi)c^2\cos(m\pi/2)} \ , \tag{15}$$

$$c = \sin\frac{n\pi}{2} \ . \tag{16}$$

We now specialize to the half-filled case, $n=1$. The condition for full spin polarization ($m=1$) resulting from Eq. (15) is

$$J > J_f = 2t\left[1 - \frac{U}{4t}\right] \tag{17a}$$

and the condition for onset of spin polarization is

$$J > J_0 = \frac{\pi}{3}t\left[1 - \frac{U}{2\pi t}\right] \ . \tag{17b}$$

For $J_0 = 0$, Eq. (17b) is the same as the usual Stoner criterion Eq. (2), since the density of states for the one-dimensional tight-binding chain is

$$g(\varepsilon) = \frac{1}{\pi(4t^2 - \varepsilon^2)^{1/2}} \ . \tag{18}$$

Thus, for small $U$ partial spin polarization occurs first and full spin polarization occurs for larger $J$. For

$$\frac{U}{t} = 6 - \pi \tag{19}$$

the lines defined by Eqs. (17a) and (17b) cross and the system goes directly from unpolarized to fully polarized. The situation here is somewhat different than that found for a constant density of states (Fig. 6 of Ref. 1) as the condition Eq. (15) does not yield lines that cross at the same point for different $m$'s. Figure 1 shows the critical $J$'s that result for various $m$, and Fig. 2 shows $m$ versus $J$ for various $U$ (compare with Fig. 7 of Ref. 1). Because the density of states is not constant here, the magnetization jumps discontinuously from finite $m$ to $m=1$ in certain cases. From Eq. (15) one easily sees that the magnetization goes continuously from 0 to 1 in the regime

$$U \le 2t \tag{20a}$$

while it jumps from a maximum magnetization discontinuously to 1 for

$$2t \le U \le (6-\pi)t \ . \tag{20b}$$

The maximum magnetization is given by the solution of the equation

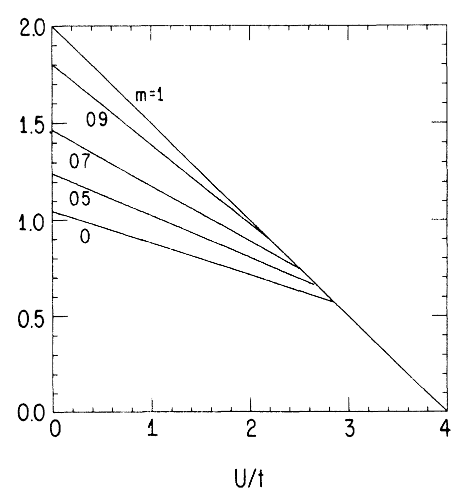


FIG. 1. Lines of constant magnetization (numbers next to the lines) within mean-field theory. The system is fully spin polarized for parameters above the line labeled $m=1$, and below the line labeled 0 the system is antiferromagnetic.

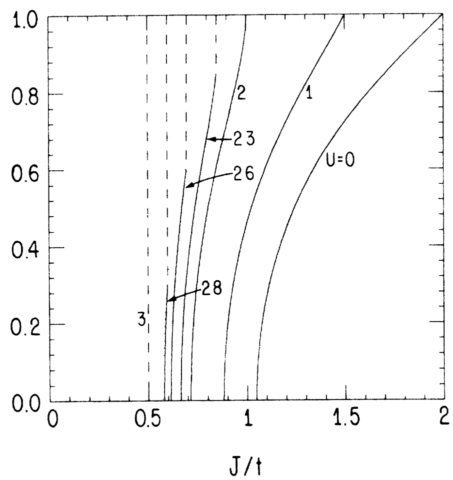


FIG. 2. Magnetization vs $J$ for various values of $U$ (numbers next to the curves) within mean-field theory. For $2 \le U/t \le 2.86$ the magnetization jumps discontinuously from a finite nonzero value to $m=1$ (this is indicated by the dashed lines). For $U/t > 2.86$ the transition is directly from $m=0$ to 1. The dotted line indicates the maximum magnetization vs $J$.

$$\frac{4}{5}\left[\frac{U}{4t}-1\right]\cos\frac{m\pi}{2}=\frac{m}{\sin(m\pi/2)}-1 \tag{21}$$

and is shown in Fig. 3 versus $U$. For $U>(6-\pi)t$ no partial spin polarization is obtained, and for $U \ge 4t$ full polarization is obtained even for $J=0$.

We can obtain an exact criterion for the stability of the fully polarized ferromagnetic state by comparing its energy with the energy of the lowest state with on overturned spin. The procedure is discussed in Ref. 5 for a general hypercubic lattice, and we repeat here some equations for completeness. A particle-hole transformation on spin-up electrons yields

$$c_{i\uparrow} \to (-1)^i c_{i\uparrow}^\dagger \tag{22}$$

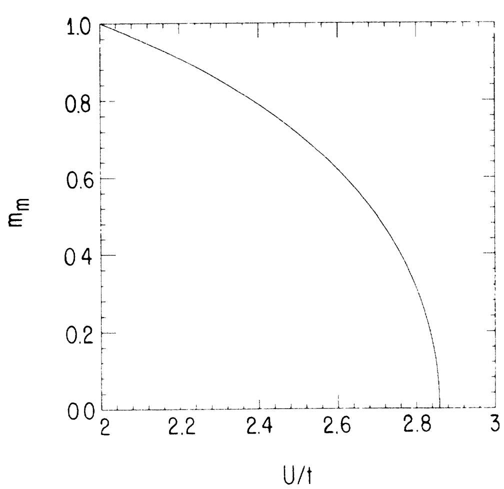


FIG. 3. Maximum partial magnetization vs $U$ within mean-field theory. The system cannot sustain a partially magnetized state with magnetization larger than $m_m$ in this parameter regime.

and the Hamiltonian Eq. (3) becomes (neglecting constants)

$$\begin{aligned} H = & -t \sum_{\substack{\langle ij \rangle \\ \sigma}} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - U \sum_i n_{i\uparrow} n_{i\downarrow} \\ & + J \sum_{\langle ij \rangle} (c_{i\uparrow}^\dagger c_{j\uparrow} c_{i\downarrow}^\dagger c_{j\downarrow} + c_{j\uparrow}^\dagger c_{i\uparrow} c_{j\downarrow}^\dagger c_{i\downarrow}) \\ & + 2J \sum_i n_{i\uparrow} + U \sum_i n_{i\downarrow} - J \sum_{\substack{\langle ij \rangle \\ \sigma}} n_{i\sigma} n_{j\sigma} . \end{aligned} \tag{23}$$

The energy of the fully polarized state is $E=0$. With one overturned spin, the energy is

$$E = E_0 + U + 2J \tag{24}$$

with $E_0$ the ground-state energy of

$$\begin{aligned} H = & -t \sum_{\substack{\langle ij \rangle \\ \sigma}} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - U \sum_i n_{i\uparrow} n_{i\downarrow} \\ & + J \sum_{\substack{\langle ij \rangle \\ \sigma}} (c_{i\sigma}^\dagger c_{j\sigma})(c_{i,-\sigma}^\dagger c_{j,-\sigma}) \end{aligned} \tag{25}$$

with one $\uparrow$ and one $\downarrow$ particle. The second term in Eq. (25) describes an attractive interaction between the hole and the overturned spin and the last term describes a "pair hopping" of the hole together with overturned spin. The condition for full spin polarization is then

$$E_0 + U + 2J > 0 . \tag{26}$$

We construct the wave function

$$|\psi\rangle = \sum_{i,l} f(l) c_{i\uparrow}^\dagger c_{i+l\downarrow}^\dagger |0\rangle \tag{27}$$

and application of the Hamiltonian leads to the equation for the coefficients

$$-2t[f(l+1)+f(l-1)] + \delta_{l,0}(2J-U)f(l) = E_0 f(l) . \tag{28}$$

Introducing the Fourier-transformed amplitudes

$$f(l) = \sum_k e^{ik\cdot l} f_k , \tag{29}$$

Eq. (28) yields

$$f_k = (2J-U)\frac{1}{N}\frac{1}{E_0+4t\cos k}F_0 \tag{30}$$

with

$$F_0 = \sum_k f_k . \tag{31}$$

Summing over $k$ then leads to the condition for the eigenvalues

$$1 = (2J-U)\frac{1}{N}\sum_k \frac{1}{E_0+4t\cos k} . \tag{32}$$

If $E_0$ is inside the band this equation can be satisfied with $E_0$ differing by $O(1/N)$ from $-4t\cos k$ for any given $k$, which correspond to scattering states. The lowest-energy scattering state has energy [within $O(1/N)$]

$$E_0 = -4t \tag{33}$$

and yields the lowest-energy state in the regime

$$2J - U > 0 \ . \tag{34}$$

The condition Eq. (26) becomes

$$J > 2t \left[ 1 - \frac{U}{4t} \right] \tag{35a}$$

which is identical to the condition obtained from mean-field theory for full spin polarization [Eq. (17a)]. Due to the condition (34), Eq. (35a) is only valid in the regime

$$U \leq 2t \ . \tag{35b}$$

When Eq. (34) is not satisfied, a solution to Eq. (32) exists where the lowest eigenvalue is below the bottom of the band, $E_0 < -4t$, describing a bound state where the hole and the overturned spin propagate tightly coupled. Equation (32) is simply evaluated by contour integration and yields

$$E_0 = -[(U-2J)^2 + (4t)^2]^{1/2} \ . \tag{36}$$

Equation (36) and the condition for ferromagnetism Eq. (26) then yield the condition

$$J > \frac{2t^2}{U} \tag{37a}$$

which is remarkably the same as the condition obtained in the strong-coupling limit discussed at the beginning of this section. Equation (37a) applies in the regime

$$U \geq 2t \tag{37b}$$

and matches smoothly the condition Eq. (35) at $U = 2t$.

In the regime $U \leq 2t$ the hole and the overturned spin are not bound, which implies that the system is metallic. This is likely to be the case for other partially magnetized states with more overturned spins also.

In the regime $U > 2t$ the hole and the overturned spin are bound with a finite coherence length. From Eqs. (29) and (30) we obtain

$$f(l) \propto \frac{1}{\{[1+(U-2J/4t)^2]^{1/2} + (U-2J/4t)\}^l} \sim e^{-l/\xi} \tag{38}$$

and the coherence length is given approximately by $\xi \sim 4t/(U-2J)$. Along the phase transition line Eq. (37a)

$$\xi \sim \frac{4t}{U - (4t^2/U)} \tag{39}$$

so that the coherence length decreases rapidly from infinity as $U$ increases beyond $2t$: for example, $\xi = 4.4$ for $U = 2.5t$, and $\xi = 1.3$ for $U = 4t$. The fact that pairs occupy a finite coherence length indicates that at the transition line it will become advantageous to overturn more than a single spin, as their energies will simply add if the wave functions are nonoverlapping. As the density of overturned spins becomes large enough that pairs start to overlap, interactions will prevent further spins from overturning. Thus, this picture indicates that the magnetization jumps discontinuously from $m = 1$ to a finite value as the transition line is crossed in the regime $U \geq 2t$, the maximum partial magnetization being approximately $m_m \sim 1 - 1/\xi$. When $\xi$ approaches unity the transition will occur directly from fully polarized to unpolarized, as in the strong-coupling limit. Our results for the coherence length suggest that this is likely to occur somewhere in the range $U \sim 3t$ to $U \sim 4t$. Note that these exact results exhibit remarkable agreement with the predictions of mean-field theory.

It should be pointed out that the conditions Eqs. (35a) and (37a) only guarantee the stability of the fully ferromagnetic state with respect to a state with a single reversed spin. It is conceivable that in the regime where no bound state of a single overturned spin and hole exist, composite bound states involving more overturned spins could exist that would render the fully polarized state unstable even if Eq. (37a) is satisfied. We believe this is highly improbable but are unable to rigorously rule it out.

Finally, we find the phase boundary obtained from exact diagonalization of two sites. The energy of the singlet state is

$$E_s = \frac{U+J}{2} - \left[ \frac{(U-J)^2}{4} + 4t^2 \right]^{1/2} \tag{40a}$$

and that of the triplet state

$$E_t = -J \tag{40b}$$

yielding as the condition for ferromagnetism

$$\frac{J}{\sqrt{2}t} > \left[ 1 + \frac{U^2}{8t^2} \right]^{1/2} - \frac{U}{\sqrt{8}t} \ . \tag{41}$$

In Fig. 4 we plot the result Eq. (41) for the two-site chain and the result Eqs. (35) and (37) for the infinite chain. For two sites no partial spin polarization can exist so that the dashed line may also be interpreted as the condition

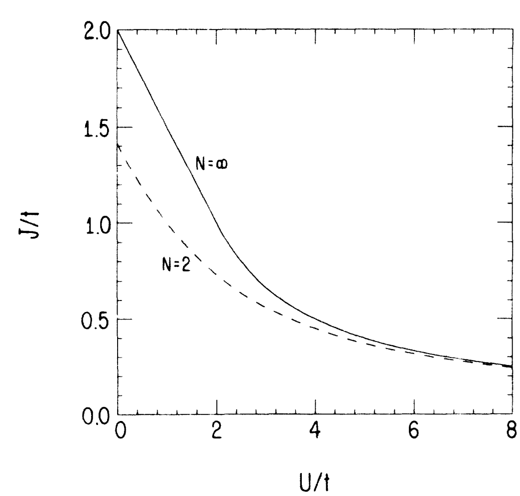


FIG. 4. Exact phase boundaries for full spin polarization for two sites and for an infinite chain.

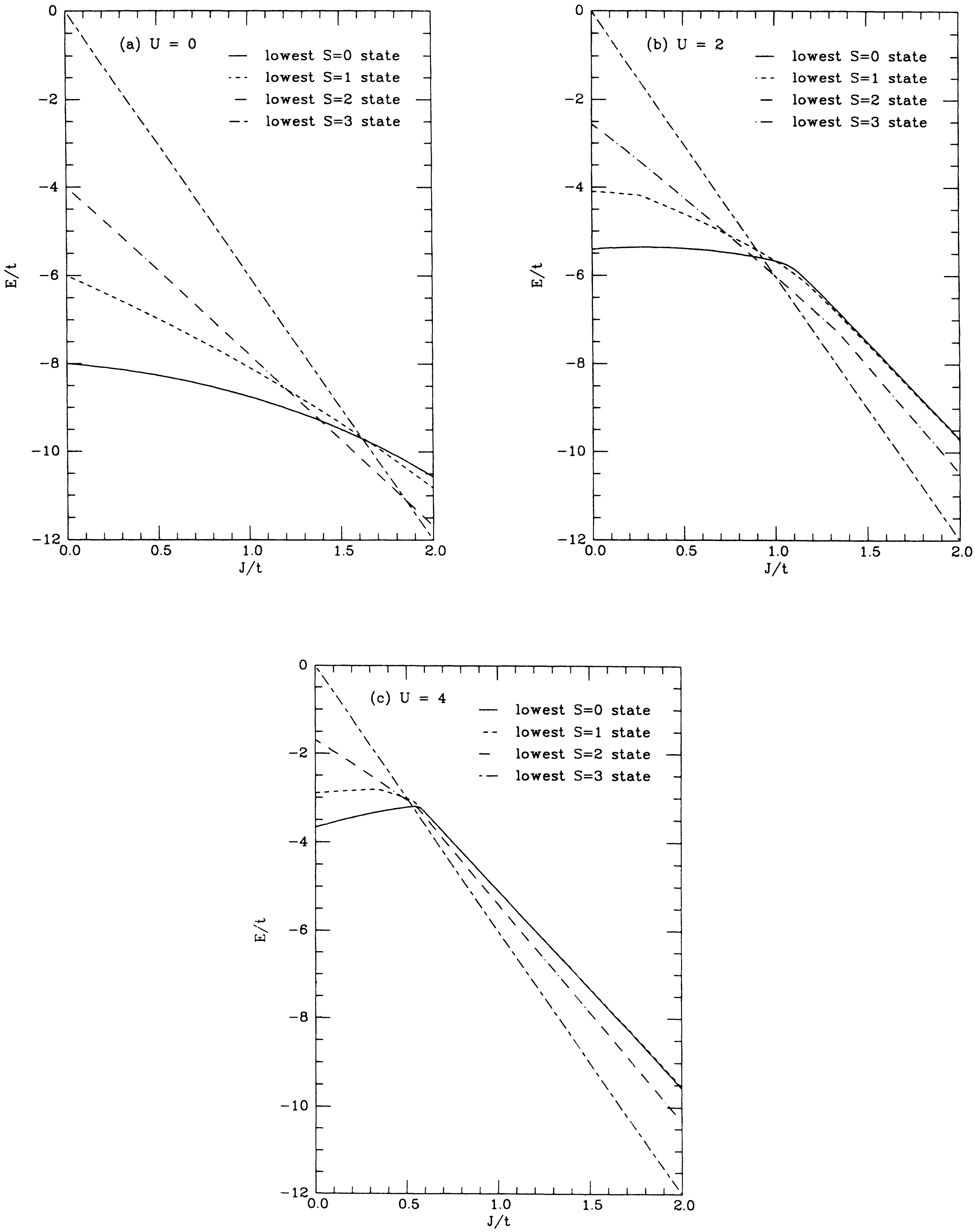


FIG. 5. Ground-state energy vs $J$ for a six-site chain for all values of the total spin $S$ allowed for $U=0$, 2, and 4. For small $J$ the ground state is always a singlet, $S=0$. Note that the value of $J$ required for spin polarization decreases as $U$ increases, and that the range in $J$ where the ground state is partially polarized shrinks as $U$ increases and has vanished at $U=4$.

for onset of spin polarization. Note the qualitative similarity of these results with the predictions of mean-field theory, Fig. 1.

## III. NUMERICAL RESULTS

We have diagonalized the Hamiltonian Eq. (3) on finite lattices using a standard diagonalization routine for $N \leq 6$ and a Lanczos algorithm for $N=8$ and 10. We use periodic (antiperiodic) boundary conditions for $N=4n+2$ ($N=4n$) sites, with $n$ an integer. This ensures that the ground state in the noninteracting case is nondegenerate and yields smooth behavior as a function of lattice size.

Figure 5 shows the ground-state energy versus $J$ for $N=6$ and spin values $S=0-3$ for various values of $U$. Note that the ground state with $S=1$ is never the lowest-energy state. For $U=0$ the system is unmagnetized for small $J$ ($S=0$), it becomes partially magnetized ($S=2$) at $J=1.39$, and fully magnetized at $J=1.85$. As $U$ increases the regime of partial spin polarization shrinks to $0.88 < J < 1.00$ for $U=2$. At $U=4$ no partial spin polarization exists. Figure 6 shows the phase boundaries for the six-site chain. The maximum $U$ where partial spin polarization exists is approximately $U=3.0$.

Similar results are found for an eight-site chain. We perform a Lanczos diagonalization starting with a random vector and measure that total spin of the obtained ground state. Figure 7(a) shows the results for $U=1$. The ground-state spin shifts from $S=0$ to 2, 3, and 4 monotonically with $U$. In contrast, in Fig. 7(b), with $U=2$, only $S=0$ 2, and 4 are obtained. Note that this behavior agrees with the mean-field prediction that for increasing $U$ the magnetization jumps discontinuously from partial to full. The phase boundaries in this case for partial and full polarization are shown in Fig. 8.

To summarize, we plot in Fig. 9 the phase boundaries for full spin polarization for $N=4$, 6, 8, 10, and $\infty$ sites,

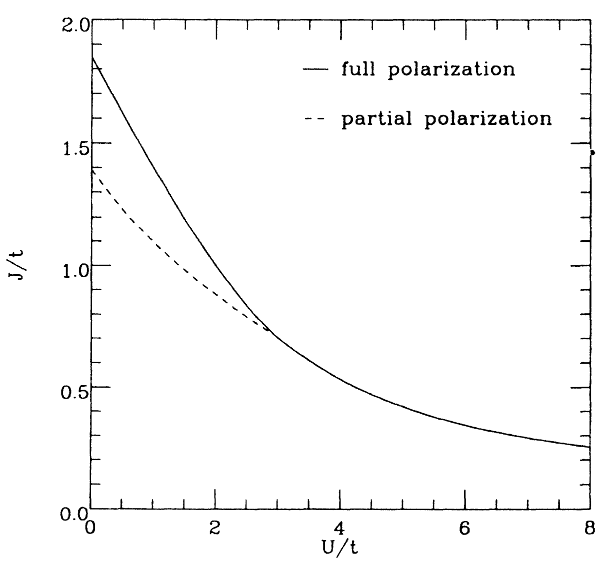


FIG. 6. Phase boundaries for onset of partial spin polarization and full spin polarization in the six-site chain.

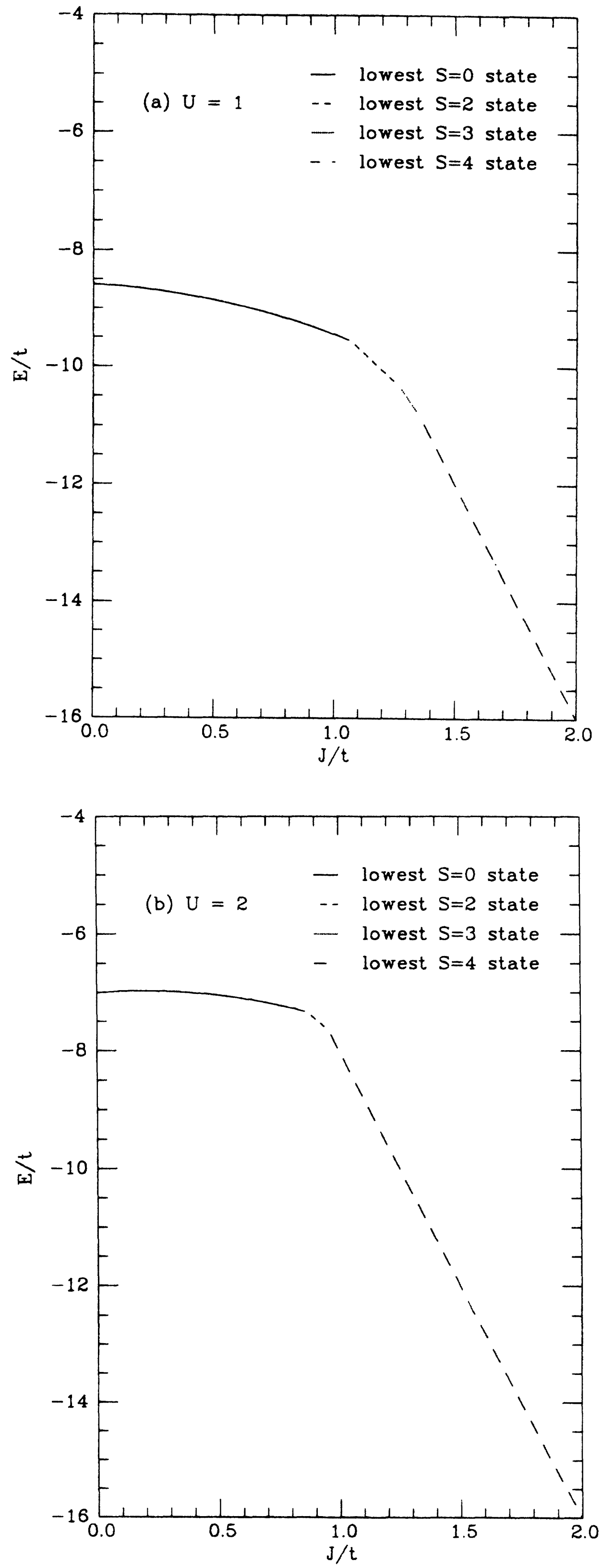


FIG. 7. Ground-state energy and spin quantum number in the ground-state vs $J$ for an eight-site chain and $U=1$ and 2. The ground state never has spin $S=1$, as in the six-site case. Note that for $U=2$ the magnetization jumps from $S=2$ to 4, in qualitative agreement with the mean-field prediction.

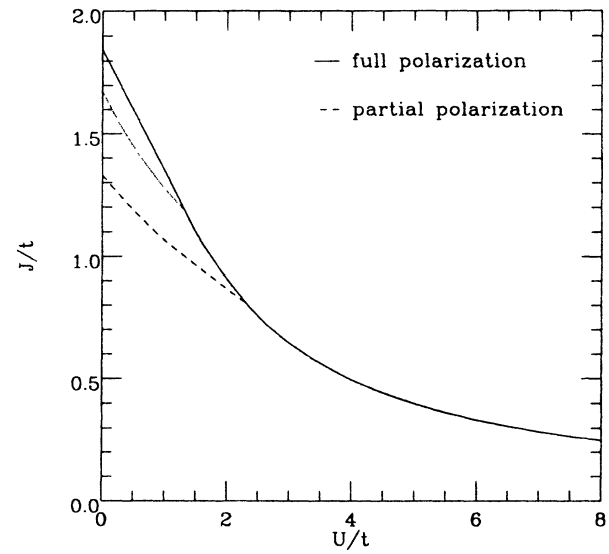


FIG. 8. Phase boundaries for onset of spin polarization ($S=2$) (dashed line) for increased partial polarization ($S=3$) (dotted line) and for full polarization ($S=4$) (solid line) in the eight-site chain.

and in Fig. 10 the boundaries for onset of spin polarization for $N=6$, 8, and 10. It can be seen that the behavior for the different lattice sizes is quite similar, and based on this we conclude that the conditions found for onset of spin polarization on the finite lattices are likely to be close to the boundary for onset of polarization in the infinite chain.

## IV. DISCUSSION

We have studied the conditions on the parameters that give rise to ferromagnetism in the model Hamiltonian Eq.

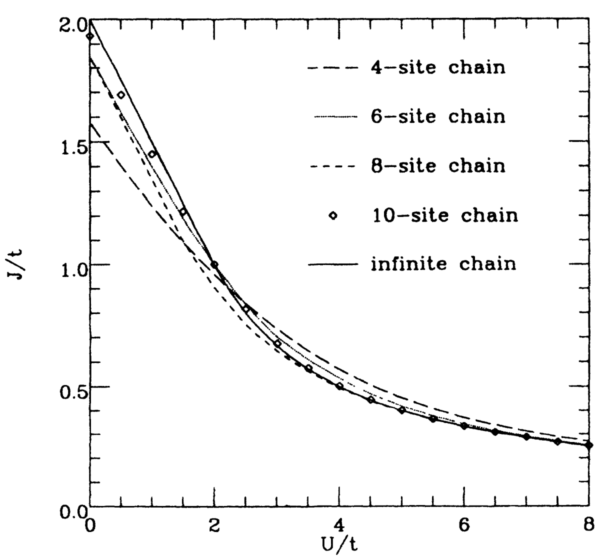


FIG. 9. Phase boundaries for full spin polarization for $N=4$, 6, 8, 10, and $\infty$.

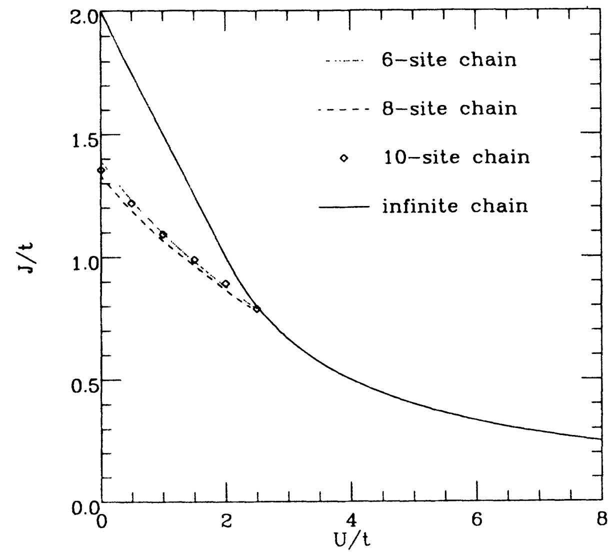


FIG. 10. Phase boundaries for onset of spin polarization for $N=6$, 8, and 10.

(1) for a one-dimensional half-filled band. Let us summarize our findings.

(1) The critical $J$'s both for onset and full polarization are decreasing functions of $U$, that approach zero as $U\rightarrow\infty$. That is, no ferromagnetism exists in our model unless $J>0$.

(2) The critical $J$ for full spin polarization coincides with the strong-coupling limiting form $J_c=2t^2/U$ for all $U\geq 2t$. For $U<2t$, it is given by $J_c=2t(1-U/4t)$ which is the result obtained from mean-field theory.

(3) A regime of partial spin polarization exists for $U$ less than a maximum value $U_c$. From our finite-lattice results we estimate $U_c/t\sim 3$.

(4) For small $U$ the magnetization increases monotonically from 0 to 1 with increasing $J$, while for $U/t>2$ it jumps discontinuously from a maximum magnetization

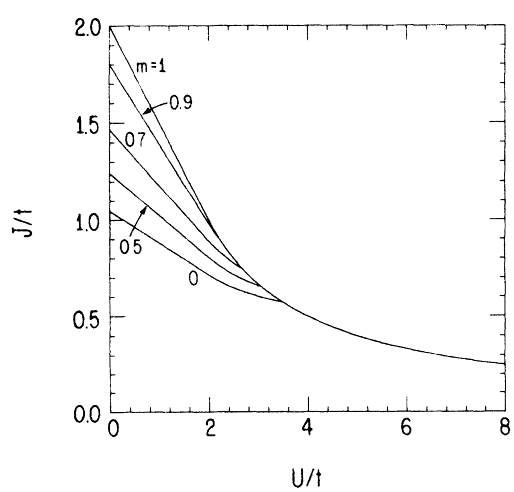


FIG. 11. Lines of constant magnetization within mean-field theory using an effective $U$ defined by Eq. (42) in the mean-field equations.

$m_m$ to 1. $m_m$ tends to 1 as $U \rightarrow U_c$.

(5) Mean-field theory qualitatively reproduces the general features obtained from the exact treatments. In particular, it correctly predicts that the magnetization goes continuously from 0 to 1 in the regime $0 \leq U \leq 2t$ and that a jump in the magnetization occurs for larger $U$. The value of $U$ where the jump becomes 1, i.e., where the transition is directly form unpolarized to fully spin polarized, is $U/t = 6 - \pi$ in mean-field theory, in reasonable agreement with the results of finite-lattice calculations.

An important goal of our study was to determine the accuracy of mean-field theory for a Hamiltonian of the form Eq. (1) in a simple case where exact solutions could be found. It is reasonable to infer that mean-field theory would yield comparably good results in other cases with this Hamiltonian. Comparison with the exact diagonalization results shows that mean-field theory underestimates the required $J$ to give rise to spin polarization by approximately 30%. As expected, mean-field theory grossly overestimates the effect of $U$ for large $U$. From comparison with the exact results we conclude that defining an "effective $U$" in the mean-field equations

$$U_{\text{eff}} = U, \quad U \leq 2t , \tag{42a}$$

$$U_{\text{eff}} = 4t(1 - t/U), \quad U > 2t , \tag{42b}$$

would give a qualitatively correct picture, as shown in Fig. 11. More generally, any smooth interpolation with the asymptotic behavior given by Eq. (42) for small and large $U$ may be expected to give a reasonable estimate of the phase boundaries. Using an effective $J$ somewhat smaller than the bare $J$ would bring the mean-field results in close agreement with the exact diagonalization results.

## ACKNOWLEDGMENTS

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