# Finite-size effects and unsaturated ferromagnetism of two-component Hubbard rings in a strong magnetic field: Exact results

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We consider two-component Hubbard models in a strong magnetic field to reveal finite-size effects in the stability of the fully polarized state against one- and two-spin flips. Also established are the criteria for unsaturated ferromagnetism, with $S_{\max}$ and $S^z$ reduced, depending on the relative signs of hopping parameters. The behavior of the critical field for periodic chains with arbitrary length at half filling is driven by Coulomb interaction, lattice frustration, and crucially band curvature. Unsaturated ferromagnetism, reminiscent of Nagaoka-like behavior, and the influence of spin liquid states are examined in the structure of off-diagonal spin correlations at large $U$. [S0163-1829(96)05720-7]

## I. INTRODUCTION

The great interest in lattice models of strongly correlated fermions comes from the belief that magnetic ordering, Mott-Hubbard, and high-$T_c$ superconductivity phenomena are contained in the direct competition between band and localization tendencies of electronic behavior. With the recent progress made in the technology of developing superparamagnetic mesoscopic systems such as rhodium clusters (which exhibit ferromagnetism not seen in bulk), high-$T_c$ materials such as $(VO)_2P_2O_7$ and $Sr_2Cu_4O_6$ weakly coupled with arrays of transition metal ladders, and the discovery of superconductivity and ferromagnetism in doped fullerenes, much attention has turned to Hubbard-like models on finite clusters of rings, chains, spheres, arrays of cubes, etc.[1] Cluster analyses for an arbitrary number of sites must in general be handled by numerical methods.[2] The reliability of numerical simulations is quite often not so obvious.

In this paper we shall focus upon simple modifications in the usual Hubbard model that generalize to a multicomponent band or orbital structure. This allows us to interpolate between a closely related family of models. The Falicov-Kimball (FK) model is characterized by one flat band and one conduction band.[3] The model with an attractive interaction between particles and holes in bands of opposite curvature is known as the excitonic model.[4] We will come to understand fully the conditions for and the nature of ferromagnetism when both finite-size effects and orbital structure are accounted for in a unified fashion. As we work with periodic chains at half filling ($n=1$), we expect an instability in the fully saturated ground state at any finite $U$. The stability of the Nagaoka state[5] in the $U\to\infty$ limit away from $n=1$ was shown to be strongly dependent on the parity in both the number of holes and atomic sites as well as the sign of the hopping term for finite lattices.[6] At exactly $n=1$ there should still be a strong role played by lattice frustration or parity on the magnetism of the ground state at finite $U$.

We present exact and analytic results concerning conditions for unsaturated ferromagnetism in Hubbard models generalized to a two-orbital band structure in half-filled rings. By unsaturated we mean maximum spin ground states $S_{\max}$ with reduced $S^z$. The problem is simplified considerably if the system is placed in a strong magnetic field:[7]

$$H=-\sum_{\langle i,j\rangle,\sigma} t_\sigma c^\dagger_{i,\sigma}c_{j,\sigma}+U\sum_i n_{i,\uparrow}n_{i,\downarrow}-\frac{h}{2}\sum_{i,\sigma}\sigma n_{i,\sigma}. \tag{1}$$

The index $\sigma$ refers to the two species of fermions. They can represent spin indices for $S=\frac{1}{2}$ electrons or orbital indices for two-component fermions. The first term is the nearest-neighbor hopping and it is spin dependent. Although $H$ no longer commutes with $S^2$, we will show it is still possible to distinguish spin in the large-$U$ limit with one spin flip. We explicitly *do not* restrict ourselves in the values *or sign* of hopping parameter $t_\sigma$ or $U$. In this way we interpolate between the various well-known systems. When $t_1=t_2>0$ we regain the Hubbard system. When $t_1$ or $t_2$ vanishes then (1) is a FK model. In allowing for negative amplitudes, the case $t_1=-t_2$ can be considered as a nonrelativistic analog for massless fermions in a Luttinger model.[8] The Coulomb parameter $U$ in the second term may also be attractive or repulsive. The external field $h$ separates the centers of the bands for each species.

The two-orbital generalization introduces an additional frustration effect. One (referred to as topological frustration) comes from the nonbipartite structure of odd $N$ rings, where $N$ is the number of sites in the ring.[6] Another effect comes from the difference in sign of hopping parameters for the two species. This we refer to as orbital frustration, and it is responsible for a distinct magnetic phase that we identify as the unsaturated ferromagnet. Additional properties of this phase will be viewed as well in the behavior of spin correlations describing off-diagonal long-range ordering (ODLRO) in the system. We show that spin liquid behavior coming from lattice frustration acts to reduce the degree of ordering and the combination of frustration effects distinguishes clearly the presence of the new phase. Finite-size

 

effects manifest in the condition for ferromagnetic instability and will be shown to be strongly suppressed depending on $U$.

The studies here consist of analyses of three questions. First is the existence of a critical field for arbitrary sign and values of $t_1,t_2$, below which the fully saturated state becomes unstable. At $n=1$, we can always expect to obtain a finite critical field, although the behavior will depend the level of frustration in the system. We calculate the critical field for a two-component model using periodic finite chains for any $U>0$. From this we come to the second question. Namely, how does the critical field depend on ring size and interaction? By analyzing exact results for small rings we find a finite-size effect on the relative stability of the fully polarized state. This effect is intrinsic to the properties of closed chains and will not be observed in the thermodynamic limit. Large-$U$ suppresses finite-size effects for stability depending on orbital frustration. The question of the symmetry of the spin wave function at large $U$ is then studied. This is shown to be a global property of the system and persists in the thermodynamic limit. This distinguishes the behavior from the Nagaoka ground state, which has been proven to exist at finite doping, and an interaction only for special bipartite lattices.[9] Also investigated is the question of the order of the transition.

The paper is organized as follows. In Sec. II we present exact results for the spectrum and phase diagram of the two-site cluster. Also given will be results concerning the ground state at the critical field of three- and four-site clusters. In Sec. III we support our conjecture regarding the symmetry and parity effects on the the ground state of our model in a critical field for closed clusters with $N$ sites. We also calculate the exact critical field for the infinite chain and compare it at $t_1=t_2$ with known results for the Hubbard model. In Sec. IV we look at the problem of a single spin flip for large $U$ in more detail by calculating off-diagonal spin correlation functions and then proceed to show that the transition is smooth by comparing it to the critical field for two spin flips at large $U$.

## II. EXACT EFFECTIVE HAMILTONIAN FOR TWO-SITE CLUSTER

An exact decoupling of charge and spin states for a two-site cluster will clearly exhibit the spin symmetries that we expect to see for arbitrary chains. We begin with the two-component Hubbard Hamiltonian on the cluster

$$H=-t_1(c_{1\uparrow}^{\dagger}c_{2\uparrow}+hc)-t_2(c_{1\downarrow}^{\dagger}c_{2\downarrow}+hc)+U(n_{1\uparrow}n_{1\downarrow}+n_{2\uparrow}n_{2\downarrow})-\frac{h}{2}\sum_{i=1,\sigma}^{2}\sigma n_{i,\sigma}, \tag{2}$$

where we allow the hopping amplitudes $t_1,t_2$ to be either positive or negative. Periodic boundary conditions on a two-site cluster will simply rescale $t\rightarrow 2t$. The coulomb parameter $U$ may be either repulsive or attractive. It is convenient to symmetrize the hopping parameters

$$\kappa_1=\frac{t_1+t_2}{2},\quad \kappa_2=\frac{t_1-t_2}{2}.$$

The Hamiltonian (2) can be transformed exactly by eliminating terms that represent mixing of spin and charge states. We move to the Hubbard representation[10]

$$c_{i\sigma}^{\dagger}\equiv X_i^{2-\sigma}+\sigma X_i^{\sigma 0},\quad c_{i\sigma}\equiv X_i^{-\sigma 2}+\sigma X_i^{0\sigma}. \tag{3}$$

Let us define the operators

$$\begin{aligned}
B_1&=\tfrac{1}{2}\sum_{\sigma}\sigma(X_1^{\sigma 0}X_2^{-\sigma 2}+X_2^{\sigma 0}X_1^{-\sigma 2}),\\
B_2&=\tfrac{1}{2}\sum_{\sigma}(X_1^{\sigma 0}X_2^{-\sigma 2}+X_2^{\sigma 0}X_1^{-\sigma 2}),\\
\tau_1&=\sum_{\sigma}X_2^{\sigma 0}X_1^{0\sigma}+X_1^{2-\sigma}X_2^{-\sigma 2},\\
\tau_2&=\sum_{\sigma}\sigma(X_2^{\sigma 0}X_1^{0\sigma}+X_1^{2-\sigma}X_2^{-\sigma 2}).
\end{aligned} \tag{4}$$

The adjoints of the above operators are obtained by reversing the order of the products of the $X$ operators that appear and also the order of the superscript indices. The $B$ and $B^{\dagger}$ operators represent interconfigurational terms that decrease and increase the number of doubly occupied sites by one unit, respectively. The $\tau$ operators conserve the number of empty and doubly occupied sites and will not contribute when the cluster is half filled. The transformation matrix can be written in the form

$$T=1-\sum_{\alpha=1,2}v_{\alpha}(B_{\alpha}^{\dagger}-B_{\alpha})+\sum_{\alpha=1,2}(u_{\alpha}-1)(B_{\alpha}^{\dagger}B_{\alpha}+B_{\alpha}B_{\alpha}^{\dagger}). \tag{5}$$

Unitarity $TT^{-1}=1$ requires $u_{\alpha}^{2}+v_{\alpha}^{2}=1$. The conditions that eliminate mixing are

$$-2\kappa_{\alpha}(u_{\alpha}^2-v_{\alpha}^2)+Uu_{\alpha}v_{\alpha}=0. \tag{6}$$

The Hamiltonian can now be written in the spin representation, appropriately projected to yield the ground-state wave function for non-negative $U$:

$$\begin{aligned}
H_{\rm eff}&=J_{\parallel}(S^z(1)S^z(2))+J_{\perp}(S^x(1)S^x(2)+S^y(1)S^y(2))\\
&\quad+\frac{(E_1+E_2)}{4}-h(S^z(1)+S^z(2)),\\
J_{\parallel}&=-(E_1+E_2),\quad J_{\perp}=-(E_1-E_2).
\end{aligned} \tag{7}$$

We have used

$$E_{\alpha}(U,\kappa_{\alpha})=\frac{U}{2}-({\rm sgn}U)\left(4\kappa_{\alpha}^2+\frac{U^2}{4}\right)^{1/2},$$

$$S^z=\tfrac{1}{2}\sum_{\sigma}\sigma X^{\sigma\sigma}=\tfrac{1}{2}\sum_{\sigma}\sigma n_{\sigma},$$

$$S^{+}=X^{\uparrow\downarrow}=c_{\uparrow}^{\dagger}c_{\downarrow},\quad S^{-}=X^{\downarrow\uparrow}=c_{\downarrow}^{\dagger}c_{\uparrow}.$$

The spin operators may be thought of as those of the original fermions in the Hilbert projected space of one electron per site.

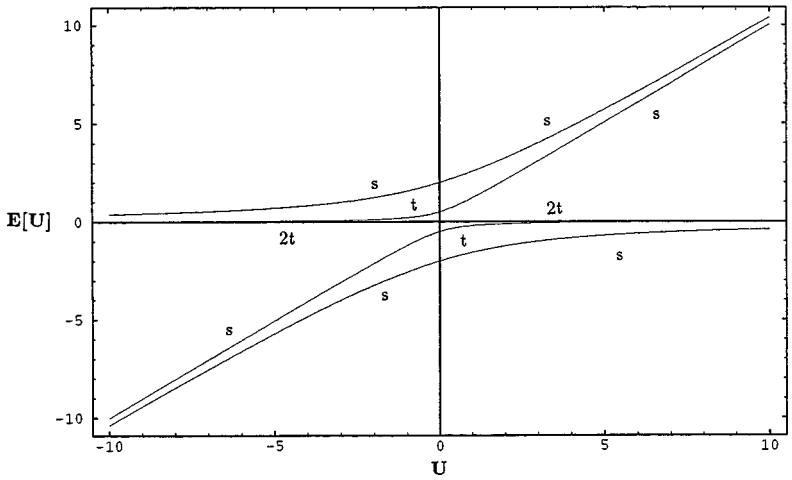


FIG. 1. Spectrum for a two-site cluster in the Hubbard regime $t_1t_2>0$. States $s$ refer to a singlet and $t$ refer to a triplet.

We regain the Hubbard limit when $\kappa_2=0$ and obtain the well-known isotropic Heisenberg antiferromagnetic model with exact exchange coupling $-E_1$. When $\kappa_1=\kappa_2$ (corresponding to the FK model), we obtain a classical Ising antiferromagnet with exchange $-2E_2=-2E_1$. The sign of $J_\perp$ is determined completely by the sign of the product $t_1t_2$. The case when $\kappa_1$ vanishes yields an orbitally frustrated Heisenberg model that may be brought to the form of the standard spin model with exchange $-E_2$, by a rotation of one of the spins by $\pi$ about the $z$ axis. The general $t_1,t_2$ model for $n=1$ is clearly an anisotropic antiferromagnetic Heisenberg model.

We identify the Hubbard-like regime as $t_1t_2>0$. In this region, the full spectrum is shown in Fig. 1. We chose to set $t_1=1$, $0\leqslant t_2\leqslant 1$, and $h=0$. Similarly, the spectrum when $t_1t_2<0$, $t_1=1$, $0\leqslant -t_2\leqslant 1$, and $h=0$ is shown in Fig. 2. Results for the ground-state wave functions with repulsive $U$ are summarized thusly:

$$t_1t_2>0,\quad |GS\rangle=\frac{1}{\sqrt{2}}\,(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle),\quad S=0,\quad E_{\mathrm{GS}}=E_1, \tag{8a}$$

$$t_1t_2<0,\quad |GS\rangle=\frac{1}{\sqrt{2}}\,(|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle),\quad S=1,\quad E_{\mathrm{GS}}=E_2. \tag{8b}$$

The spin functions here represent the dominant component of the ground-state wave function of the original system in the limit of large $U$. The spin symmetry is either the pure reduced spin singlet ($S=0$) or the unsaturated ferromagnetic state ($S=1$) and we predict the same type of behavior to be displayed for any $N$ site ring including the thermodynamic limit with one spin flip. The total spin quantum number $S$ of the spin component of the ground-state wave function remains well defined. Eigenvalues of operator $S^2$ acting on the ground state of the two-site cluster for any $U$ in the fermion representation are reduced to $\sqrt{1-\eta^2}S(S+1)$, with $S$ given above and $\eta^2$ giving the probability of a double occupancy. Crossover in the spin symmetry of the ground state occurs at $U=0$ when $t_1t_2<0$ (shown in Fig. 2) and for the FK model $t_1t_2=0$ with $U>0$ (Fig. 3). When $U$ is attractive, the ground state is always of the bosonic (paired) type and is a spin singlet. This is shown in Fig. 4. Henceforth we consider only repulsive potentials.

From Eqs. (8) we can immediately see the direct effect of orbital frustration upon symmetry of the ground-state spin

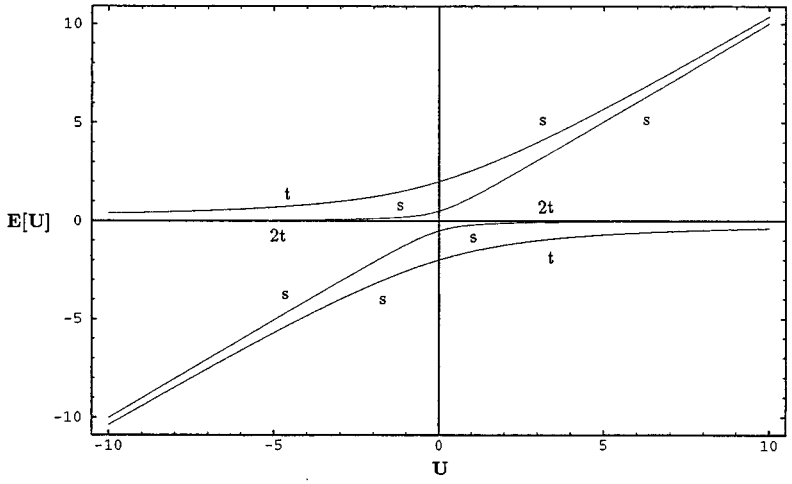


FIG. 2. Spectrum for a two-site cluster in the orbitally frustrated regime $t_1t_2<0$.

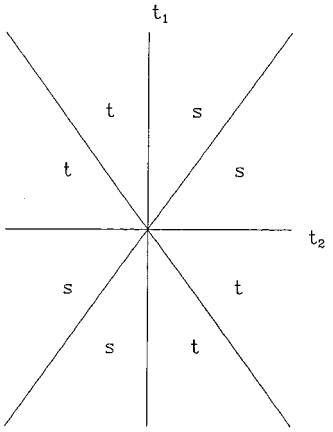


FIG. 3. Ground-state phase diagram for a two-site cluster when $U>0$.

wave function. If we introduce a strong magnetic field $h$, then the saturated ferromagnetic ground state with maximum $S$ (Nagaoka state) becomes unstable when the field is lowered to its critical value:

$$h_c=\sqrt{4(|t_1|+|t_2|)^2+U^2/4}-U/2. \tag{9}$$

Here we invoke periodic boundary conditions on the cluster. The transition reduces the total spin if $t_1t_2>0$ and preserves maximum spin when orbitally frustrated $t_1t_2<0$. By breaking the rotational symmetry of the model, we allow the system to maintain the spin symmetry of the Nagaoka state while reducing the $S^z$ component.

Similar behavior for any $N$ will appear in the symmetry properties of the component of the ground-state wave function with double occupancies projected out in a strong field. This was checked explicitly for $N=3,4$ sites. When $N=3$, we have for the projection at large $U$ of the single spin flip ground state with one electron per site

$$t_1t_2>0, \quad S=\tfrac{1}{2}, \quad S^z=\tfrac{1}{2}, \tag{10a}$$

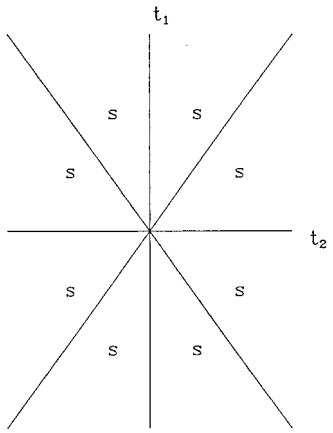


FIG. 4. Ground-state phase diagram for a two-site cluster when $U<0$.

$$t_1t_2<0, \quad S=\tfrac{3}{2}, \quad S^z=\tfrac{1}{2}. \tag{10b}$$

The wave function associated with (10b) shows the expected unsaturated ferromagnetism

$$|GS\rangle=1/\sqrt{3}(|\uparrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\rangle+|\uparrow\uparrow\downarrow\rangle). \tag{11}$$

In the Hubbard regime (10a), the ground state is twofold degenerate with reduced spin. This is the finite lattice frustration effect that we will show reduces spin ordering as in a spin liquid. The critical field for the $N=3$ cluster is given at arbitrary $U$ by

$$h_c=\left[\left(\frac{3g}{4}\right)^2+\frac{gU}{4}+\frac{U^2}{4}\right]^{1/2}-\frac{U}{2}-\frac{g}{4}, \tag{12}$$

where

$$g(t_1,t_2,K)=2\sqrt{t_1^2+t_2^2-2t_1t_2\cos K} \tag{12'}$$

and momentum $K$ is to be chosen to maximize $h_c$ (or minimize energy). The special case $t_1t_2=0$ is the ground state of the frustrated Ising antiferromagnet and will not have a definite quantum number associated with total spin $S$. This mixed state at the critical field is $N$-fold degenerate, corresponding to the number of available momentum states.

For an $N=4$ site ring the single spin-flip ground-state spin quantum numbers in the strong-$U$ limit of one electron per site are

$$t_1t_2>0, \quad S=1, \quad S^z=1, \tag{13a}$$

$$t_1t_2<0, \quad S=2, \quad S^z=1. \tag{13b}$$

The projected wave function at large $U$ with one spin flip is

$$|GS\rangle=1/2(|\uparrow\uparrow\uparrow\downarrow\rangle\mp|\uparrow\uparrow\downarrow\uparrow\rangle+|\uparrow\downarrow\uparrow\uparrow\rangle\mp|\downarrow\uparrow\uparrow\uparrow\rangle). \tag{14}$$

The signs $\mp$ refer to Hubbard and orbitally frustrated regimes, respectively. The spin state remains pure, with $S$ determined strictly by the sign of $t_1t_2$. This suggests that the simple condition determining unsaturated ferromagnetism will persist for any $N$. We expect to find the origin of this effect to come from the optimizing choice for the excitation center of mass momentum $K$. Reduced spin states will result from choosing $K$ at the edge of the reduced Brillioun zone ($\pi$). Symmetric spin states will have $K=0$. We show this explicitly in Sec. III. We give now the exact critical field for the four-site ring at any $U$,

$$h_c=g\left(-\frac{a}{3}\right)^{1/2}\cos\left(\frac{\phi}{3}+\frac{4\pi}{3}\right)-U, \tag{15}$$

with

$$\cos\phi=\frac{-b}{2\left(\frac{-a^3}{27}\right)^{1/2}},$$

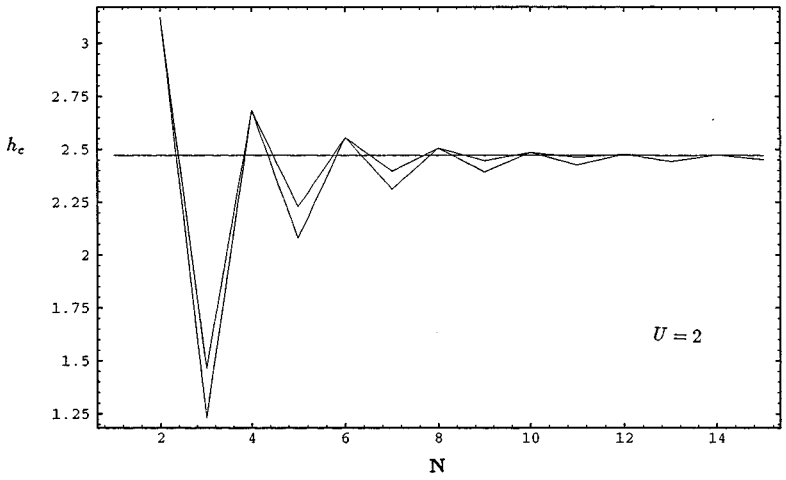


FIG. 5. Critical field $h_c$ for a single spin-flip instability of a saturated ferromagnet with $U=2$ in rings up to $N=15$. The top curve is for $t_1=t_2=-1$, while the bottom curve is for $t_1=t_2=1$. The horizontal line marks the result in the thermodynamic limit.

$$b=\frac{2\alpha}{27}\left[\alpha^2+\frac{63}{8}\right],$$

$$a=-\left(1+\frac{U}{g}\right), \quad \alpha=-\frac{U}{g}.$$

In concluding this section, we write down the effective anisotropic Heisenberg model to lowest order in parameter $t_1,t_2 \ll U$ for any lattice[11]

$$H=J_{\parallel}\sum_{\langle ij\rangle}\left[S^z(i)S^z(j)-\tfrac{1}{4}\right]+J_{\perp}\sum_{\langle ij\rangle}\left[S^+(i)S^-(j)+S^-(i)S^+(j)\right]-h\sum_i S^z(i),$$

$$J_{\parallel}=\frac{2(t_1^2+t_2^2)}{U}, \quad J_{\perp}=\frac{2t_1t_2}{U}. \tag{16}$$

All conclusions regarding spin symmetry of the single spin flipped state for any $N$ will be seen using the spin Hamiltonian (16). Since $J_{\parallel}$ is always positive, the Ising part is always antiferromagnetic.

## III. SYMMETRY AND FRUSTRATION EFFECTS FOR $N$-SITE RINGS

Let us now calculate an expression for the critical field on $N$-site closed clusters with $n=1$ for any non-negative $U$. We conjecture that the phase transition is smooth, in which case it is exact. In Sec. IV we give a real indication that this is true. So our single spin-flip ansatz for Hamiltonian (1) is

$$|\psi\rangle=\sum_{i,j}\psi_{ij}c_{j\downarrow}^{\dagger}c_{i\uparrow}|F\rangle, \tag{17}$$

with $|F\rangle=\Pi_i c_{i\uparrow}^{\dagger}|0\rangle$, and $E_F$ is the energy of the fully saturated state. Using the Schrödinger equation yields the dispersion relation. The coefficients are written

$$\psi_{ij}=\sum_{k_1,k_2}\psi(k_1,k_2)\exp i(k_1x_i+k_2x_j). \tag{18}$$

We let $k_1=\eta K-q$ and $k_2=(1-\eta)K+q$, where $K$ and $q$ are the center of mass and relative momentum coordinates, respectively. $\eta$ is a parameter to be chosen to ensure $\psi(q)=\psi(-q)$. The center of mass and relative coordinates $R=(x_i+x_j)/2$ and $r=x_i-x_j$ are defined in the usual way. The equation for $\eta$ is thus

$$t_1\tan\eta K=\frac{-t_2\sin K}{t_1-t_2\cos K}, \tag{19}$$

yielding the dispersion relation

$$-\frac{N}{U}=\sum_q \frac{1}{\epsilon-g(t_1,t_2,K)\cos q}, \tag{20}$$

where

$$\epsilon=E-U-h-E_F.$$

Bound states between the electron and hole exist if $E$ lies below the bottom of the band determined by $g(t_1,t_2,K)$. For one-dimensional rings we always have a bound state when $U>0$. The minimizing values for $K$ are given

$$t_1t_2>0, \quad K=\pi \quad \text{for } N_{\text{even}}; \quad K=\frac{N-1}{N}\pi \quad \text{for } N_{\text{odd}}; \tag{21a}$$

$$t_1t_2<0, \quad K=0 \quad \text{for all } N; \tag{21b}$$

$$t_1t_2=0, \quad K, \quad N\text{-fold degenerate}. \tag{21c}$$

In the thermodynamic limit integration of (20) yields $h_c$ when $E=E_F$:

$$h_c=\sqrt{g(t_1,t_2,K)^2+U^2}-U. \tag{22}$$

This agrees with previous results for the Hubbard model when $t_1=t_2$.[12] In Figs. 5 and 6, $h_c$ is plotted as a function of $N$ up to 15 sites for both $t_1t_2=\pm 1$ and we also include the infinite chain limit as the horizontal line. Figure 7 shows results for $t_2=0$.

There are a couple of important observations to be made in Figs. 5 and 6. We notice that $h_c$ is independent of the sign of $t_1t_2$ when the rings are bipartite. This is clear from the fact that a unitary transformation on $H$ rotates one system to the

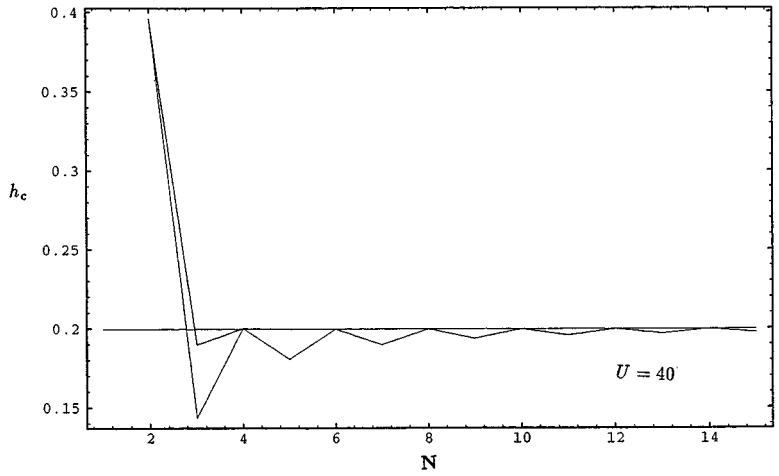


FIG. 6. Critical field $h_c$ for a single spin-flip instability of the saturated ferromagnet in a strong interaction limit with $U=40$ in rings up to $N=15$. The top curve is for $t_1=t_2=-1$, while the bottom curve is for $t_1=t_2=1$. The horizontal line marks the result in the thermodynamic limit.

other without altering the spectrum. For even rings $h_c$ gives an upper bound to the infinite chain result. Lattice frustration has two effects. It relatively stabilizes the saturated ferromagnetic ground state. When the lattice is frustrated ($N$ odd), $h_c$ is a lower bound to the infinite chain limit (hence the oscillations) and is a monotonic increasing function of $N$. It also breaks the degeneracy coming from orbital frustration. This becomes more pronounced as $U$ increases. The strongest oscillations of $h_c$ as a function of $N$ are correlated strictly with both $t_1t_2>0$ and lattice frustration. We may conclude that spin liquid states stabilize the saturated ground state. This liquidlike behavior for small $N$ is analogous to the spin liquid phase in two-dimensional antiferromagnetic triangular (frustrated) lattices.[13]

In comparing Figs. 5 and 6, it is clear that strong $U$ distinguishes orbital frustration by almost completely suppressing finite-size effects when $t_1t_2<0$. Lattice frustration plays a role only in the spin liquid regime $t_1t_2>0$ by partially stabilizing the saturated ground state. The thermodynamic limit result is reached already for all $N>3$ when $t_1t_2<0$ and for bipartite rings with $t_1t_2$ positive or negative.

The symmetry of the projected wave function with one electron per site is determined by the sign of $t_1t_2$. This can be made clear if we make a similar analysis in strong $U$ of the ground state of anisotropic Heisenberg model (16) with one spin flip. A single overturned spin behaves like a free particle, yielding the spectrum

$$E_q=E_F+h-4J_{\parallel}+8J_{\perp}\cos q. \tag{23}$$

It can be easily verified that $h_c$ obtained above agrees with Eq. (22) to lowest order. Exchange coefficients $J_{\parallel}$ and $J_{\perp}$ are given in Eq. (16). The ground-state eigenfunction is written

$$|\psi\rangle=\sum_i Ae^{iqx_i}S^-(i)|F\rangle, \tag{24}$$

where $A$ is the normalization constant. This is simply the $U\to\infty$ limit of ansatz (17). To prove that total spin quantum number remains well defined for all $t_1,t_2$, it is sufficient to show

$$S^2|\psi\rangle=S(S+1)|\psi\rangle. \tag{25}$$

One easily can verify that

$$S^2|\psi\rangle=\frac{N}{2}\left(\frac{N}{2}+1\right)|\psi\rangle, \quad q=0, \quad S=S_{\max}=\frac{N}{2}, \tag{26a}$$

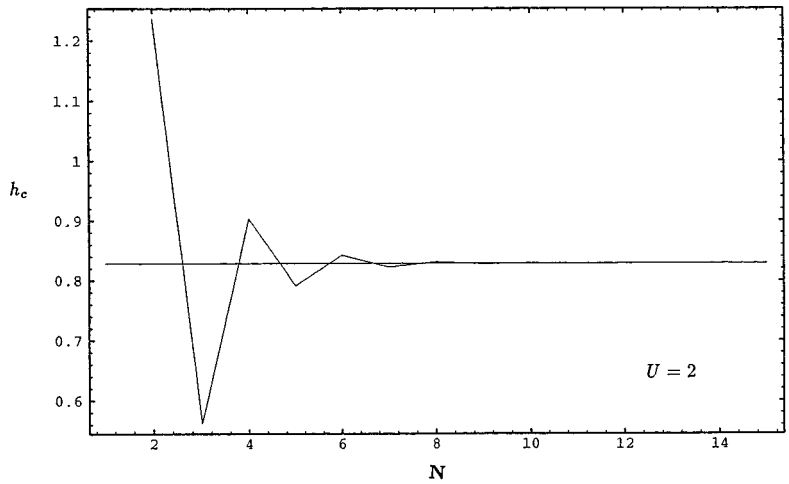


FIG. 7. Critical field for Falicov-Kimball rings with $t_2=0$ up to $N=15$ for $U=2$. The horizontal line marks the result in the thermodynamic limit.

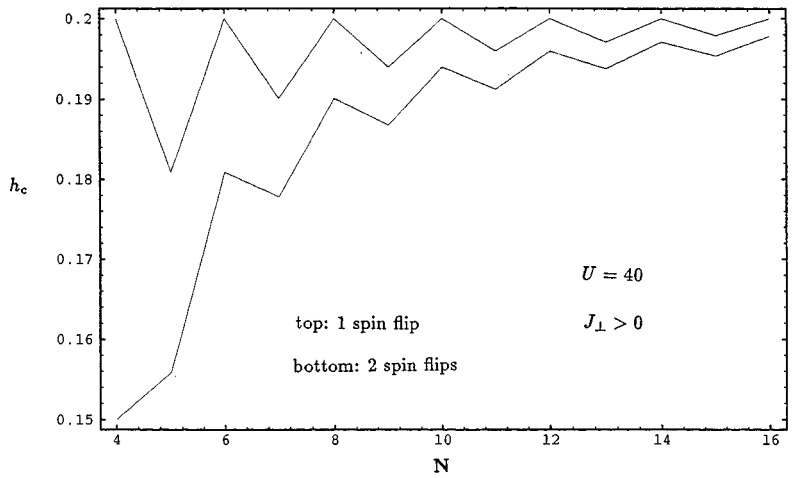


FIG. 8. Critical field for one and two spin flips with $U=40$ and $t_1=t_2=1$ in rings up to $N=16$. $h_c$ for two spin flips is below that for one spin flip, indicating a smooth transition.

$$S^2|\psi\rangle=\frac{N}{2}\left(\frac{N}{2}-1\right)|\psi\rangle, \quad q=\pi, \quad S=S_{\max}-1. \tag{26b}$$

Condition (26b) holds only for $N$ even or in the thermodynamic limit, while (26a) is true for any $N$. Thus

$$[H,S^2]|\psi\rangle=0. \tag{27}$$

Results for the ground state may be summarized as

$$J_\perp>0, \quad q=\pi \quad \text{for} \quad N_{\text{even}};$$

$$q=\frac{(N-1)}{N}\,\pi \quad \text{for} \quad N_{\text{odd}}; \quad S=S_{\max}-1, \tag{28a}$$

$$J_\perp<0, \quad q=0 \ \text{ for all } N, \quad S=S_{\max}=\frac{N}{2}. \tag{28b}$$

In the sector of states with more than one spin flip,[27] will not in general be true and we no longer have pure states. In the isotropic antiferromagnetic Heisenberg limit $J_\parallel=2J_\perp$. The total spin then becomes a good quantum number and is maximally reduced to the value $S=S_{\max}-N_f$, where $N_f$ is the number of spins flipped.

## IV. SPIN CORRELATIONS AND TRANSITION ORDER

Figure 6 gives us a picture of the strength of long-range ordering in our system when $U$ is large. As a rule, we can say that a higher $h_c$ is associated with longer-range correlations. Weaker $h_c$ is associated with reduced ordering and a stabilized saturated ground state. To see this, consider the correlation defining ODLRO in the $XY$ plane

$$c(x-y)=\langle S^+(x)S^-(y)+S^-(x)S^+(y)\rangle. \tag{29}$$

We take the expectation using the wave function in (24). One finds

$$c(x-y)\sim\frac{1}{N}\cos q(x-y).$$

The system has ferromagnetic ODLRO ($1/N$) when $q=0$, $J_\perp<0$ for all $N$. This is the unsaturated ferromagnet. Antiferromagnetic ODLRO in the $XY$ plane $(-1)^{|m-y|}/N$ exists when $J_\perp>0$ for bipartite lattices. In both cases $h_c$ converges rapidly to the $N\to\infty$ result, indicating suppression of finite-size effects. This is all consistent with our symmetry analyses of the single spin-flip wave function (24).

Lattice frustration introduces finite-size effects when $J_\perp>0$. Stabilization of $|F\rangle$ is seen in Fig. 6 and there is a

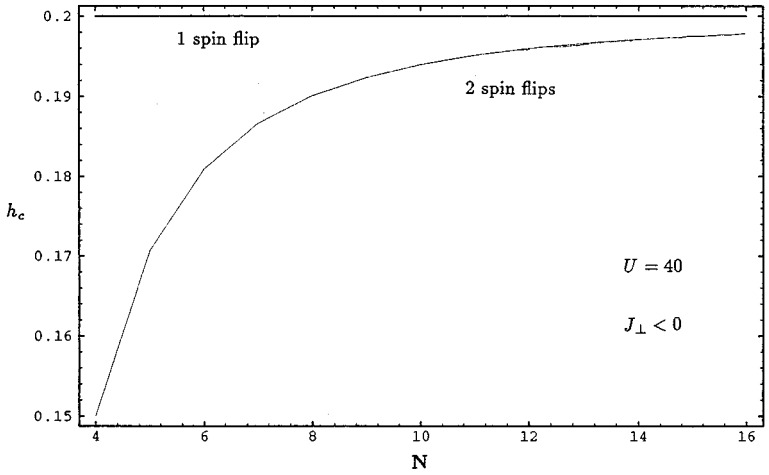


FIG. 9. Critical field for one and two spin flips with $U=40$ and $t_1=-t_2=1$ in rings up to $N=16$. $h_c$ for two spin flips again lies below that for one spin flip, indicating a smooth transition.

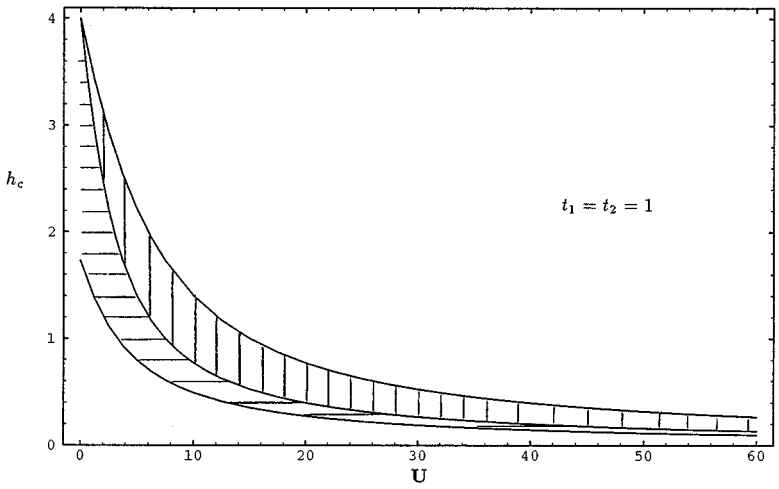


FIG. 10. Critical field as a function of $U$ with $t_1 = t_2 = 1$. The region of upper bounds (vertical shading) comes from bipartite periodic chains, whereas the lower-bound region (horizontal shading) is the spin liquid regime for odd chains.

reduction of ODLRO in the system. The correlation goes like $[(-1)^{|m-y|}/N]\cos(|z-y|\pi/N)$. This is spin liquid type behavior for nonbipartite finite lattices. In the thermodynamic limit the effect vanishes. We emphasize that the appearance of maximum spin states and unsaturated ferromagnetism, unlike spin liquid behavior, is a global property and persists when $N \to \infty$.

We now examine more closely the question of the order of the transition. The reduction of $S^z$ has thus far been assumed to be smooth (second order). Justification will come from the calculation of $h_c$ for a transition from the fully magnetized state to an eigenstate state with two spin flips. A second-order transition will have a smaller critical field associated with this case in comparison with one spin flip. Again we work in the large-$U$ limit with the anisotropic Heisenberg model (16). Our two-spin-flip ansatz is

$$|\phi\rangle = \sum_{i<j} a_{ij} S^-(j) S^-(i) |F\rangle. \tag{30}$$

The strong-coupling limit reduces what would be a four particle problem in the original fermion space to a two-body problem in the projected Hilbert space where particle and hole are fully localized. The problems are similar, only now we have to deal with essentially hard-core bosons with a nearest-neighbor repulsion, so no bound states exists. Coefficients $a_{ij}$ are written as in Bethe ansatz,

$$a_{ij} = \sum_{k_1,k_2} a(k_1,k_2)[\exp(ik_1x_i + ik_2x_j) + \exp(ik_2x_i + ik_1x_j)]. \tag{31}$$

We make sure to handle the hard-core condition by introducing diagonal coefficients $a_{ii}$ in the usual manner.[14] The following dispersion equation is obtained:

$$\frac{1}{N}\sum_q \frac{1}{\cos p - \cos q} = \frac{J_\parallel}{J_\parallel \cos p - 2J_\perp \cos\frac{Q}{2}}. \tag{32}$$

$q$ is the relative momentum, $Q$ is center of mass momentum, and

$$\cos p = \frac{\epsilon}{16 J_\perp \cos\frac{Q}{2}}, \tag{33}$$

with

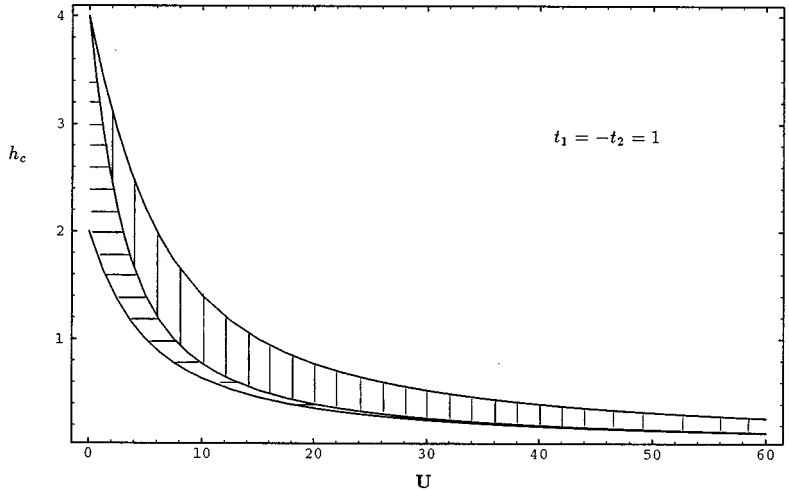


FIG. 11. Critical field as a function of $U$ for the orbitally frustrated case $t_1 = -t_2 = -1$. The region of upper bounds (vertical shading) comes from bipartite chains, whereas the lower-bound region (horizontal shading) is the unsaturated ferromagnetic regime for odd chains.

$$\epsilon = E + 8J_{\parallel} - 2h - E_F . \tag{34}$$

$Q$ is chosen to minimize the energy. The lowest energy is now above the bottom of the band shown in (32).

A plot of $h_c$ for two spin flips in rings up to $N=16$ is shown in Fig. 8 with $U=40$ and for the isotropic antifferromagnetic spin model. This is the bottom curve. The top curve is the single-spin-flip result and it shows that indeed the transition is second order. Figure 9 is the same plot, but for $J_{\parallel} = -2J_{\perp}$. Here the transition is also shown to be second order. Note that the oscillation in Fig. 8 is consistent with antifferomagnetism, while the monotonic structure in Fig. 9 is consistent with unsaturated ferromagnetism. This is a strong indication that the tendency toward maximizing total spin will remain even as the magnetic field is reduced to zero, although $S$ is no longer a good quantum number.

## V. CONCLUSION

We have investigated conditions for which both saturated and unsaturated ferromagnetism are to be found in a general two-component Hubbard model with a repulsive Coulomb interaction in a strong magnetic field. The model with $t_1 t_2 < 0$ identifies the unsaturated ferromagnet and may be relevant to the problem of orbital magnetism in heavy fermions, since electrons from two orbitals with different curvatures are participating in electronic transitions. We expect excitonic correlations in mixed valence states (analogous to the spin-flip phase) in frustrated lattices at high pressure (strong magnetic field) near the boundary to fully polarized orbitals to exhibit properties similar to the unsaturated ferromagnet. The orbitals may in this interpretation be $4s$ and $4d$ for example. Our analysis was done for periodic rings at half filling. Exact results were obtained by focusing on two-particle spectra of the system in a critical field. This critical field was determined analytically for an infinite lattice and exactly for $N$ up to 15 sites. We found that although a smooth transition to a singly spin flipped state is inevitable ($h_c \neq 0$), the dependence of the critical field on lattice frustration, orbital frustration, and $U$ reveal interesting and definitive magnetic properties. Results are summarized compactly in Figs. 10 and 11.

A distinct magnetic phase with maximal total spin states ($S_{\max}$) and reduced $S^z = S_{\max} - 1$ is obtained as the ground state when $J_{\perp} < 0$ and $U$ is large. This is true for both bipartite and nonbipartite rings and remains in the thermodynamic limit. Results here for unsaturated ferromagnetism do not conflict with the Lieb-Mattis theorem, which asserts a minimum spin ground state for chains with open boundaries, and spin-independent non-negative hopping parameters.[15] These states were found to exhibit power-law decay with off-diagonal ferromagnetic type of ordering. This phase can be found as well for both the two-site cluster and infinite chain with open boundaries. In the large-$U$ limit, finite-size effects in the behavior of $h_c$ are completely suppressed for these states. Oscillations in $h_c$ as a function of $N$ are found to characterize the ground state when $J_{\perp} > 0$, and the system exhibits a reduced total spin with antiferromagnetic ODLRO. This ordering is diminished when the lattice is frustrated, and the ground state is reminiscent of a spin liquid. Here the saturated ferromagnetic state is relatively stabilized when compared with the orbitally frustrated case. The Falicov-Kimball limit has an $N$-fold degenerate ground state in a critical field and represents the crossover between unsaturated ferromagnetism and reduced spin ground states in $t_1, t_2$ parameter space.

Future work is planned to focus on finite-size effects for arrays of two-component coupled Hubbard chains and cubes. We also plan to investigate the meaning of stability and unsaturated ferromagnetism conditions when the Coulomb interaction is attractive.


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