Ferromagnetism in the Hubbard model on a two-leg ladder with interchain Coulomb repulsion

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We investigate the ground-state magnetic properties of the Hubbard model on a two-leg ladder with interchain Coulomb repulsion. When both the on-site and the interchain Coulomb repulsions are infinitely large, we show exactly that the model exhibits saturated ferromagnetism in the ground states for the electron filling factor $1/4 < n < 1/2$. The explicit expression of the saturated ferromagnetic ground state is also obtained. By using numerical calculations, we find that ferromagnetism remains stable for sufficiently large values of these interactions, and that the interchain Coulomb repulsion induces tendencies to ferromagnetism, especially on the 1/4-filling side for small values of the interchain hopping parameter.

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I. INTRODUCTION

Ferromagnetism in itinerant electron systems has been studied by many physicists for a long time. However, there still remain open questions about microscopic mechanisms for itinerant ferromagnetism. The problem has been mostly discussed by using the Hubbard model,[1–3] the tight-binding model only with the on-site Coulomb interaction U. So far a few rigorous works[4–10] and a number of analytical and numerical works[11–14] have given evidence of itinerant ferromagnetism in Hubbard models.

Because the Coulomb interaction is a long-range interaction in real materials, it is important to clarify effects of off-site interactions on ferromagnetism. About the problem, one usually discussed the extended Hubbard model including nearest-neighbor electron-electron interactions, such as charge-charge interaction V, bond-charge interaction X, exchange interaction F, and pair hopping F'. Hirsch[15,16] and Tang and Hirsch[17] pointed out that F plays an important role in the stabilization of ferromagnetism. Kollar *et al.* derived extended Nagaoka's theorem that positive values of F lead a ground state to ferromagnetism for finite U.[18] They also showed that ferromagnetism is stable for $X=t$ (t is the hopping parameter) on lattices with loop structure even if $F=0$. As for V, Tasaki proved rigorously that an extended Hubbard model on a railway-trestle lattice has the saturated ferromagnetic ground states in the limit $U\to\infty$ and $V\to\infty$ for the electron filling factor $1/4<n<1/2$.[10] By using the density-matrix renormalization group (DMRG), Arita *et al.* investigated the effects of V on the magnetic properties of the Hubbard model on a δ chain and a railway-trestle lattice.[19] They found a region where the critical values of U, above which the system becomes ferromagnetic, are reduced in the phase diagram by V.

The nearest-neighbor Coulomb repulsion V is usually the largest among nearest-neighbor electron-electron interactions. Moreover, how ferromagnetism is affected by V is a nontrivial problem, because V is independent of spin unlike the direct exchange interaction. Nevertheless, literature concerning its effects is still limited. In this paper, we investigate the effect of the off-site Coulomb repulsion on ferromagnetism in the Hubbard model on a two-leg ladder. Hubbard models on ladder lattices are believed to describe not only essential features of various materials such as MgV_2O_5, CaV_2O_5,[20] $SrCu_2O_3$,[21] but also some properties of two-dimensional rather than one-dimensional systems. By using DMRG, Kohno showed that, in the limit $U\to\infty$, a Hubbard ladder without the off-site Coulomb repulsion exhibits ferromagnetism for sufficiently large values of the interchain hopping parameter for $1/4<n<1/2$.[22] As for an extended Hubbard ladder with the off-site Coulomb repulsion, by using DMRG, Vojta *et al.* investigated an isotropic case of $V_\parallel = V_\perp = V$ for $t_\perp/t=1$, where $V_\parallel$, $V_\perp$, $t_\perp$, and t represent parameters of the intrachain off-site repulsion, the interchain off-site repulsion, the interchain hopping, and the intrachain hopping, respectively.[23] They showed that the system goes into the charge-density wave phase as V/t is increased, but they did not furnish evidence of the stability of ferromagnetism. In this paper, we consider the anisotropic case of $V_\parallel=0$, $V_\perp=V$ for $t_\perp/t\neq 1$ as well as $t_\perp/t=1$.

This paper is organized as follows: In Sec. II, we define an extended Hubbard model with the interchain Coulomb repulsion V on a two-leg ladder. In Sec. III, we present a rigorous proof on the ground state of the extended Hubbard model in the limit $U-V\to\infty$ and $V\to\infty$. In Sec. IV, we present numerical results on ferromagnetism in the model. Section V is a summary and discussion.

II. DEFINITION OF THE MODEL

Let us define a ladder lattice Λ as

$$\Lambda=\{x=(\alpha,j)\,|\,\alpha=1,2,\quad j=1,2,\ldots,N\}, \tag{1}$$

where N is an arbitrary even integer. We impose periodic boundary conditions on Λ, so that $(\alpha,N+1)$ is identified with $(\alpha,1)$. We denote by $|X|$ the number of elements in a set X. The number of sites in Λ satisfies $|\Lambda|=2N$.

We consider an extended Hubbard model on Λ described by the following Hamiltonian (Fig. 1):

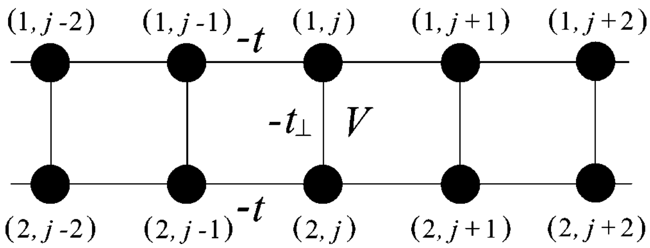

FIG. 1. The ladder lattice.

$$\begin{aligned}H=&-t_{\perp}\sum_{j=1}^{N}\sum_{\sigma=\uparrow,\downarrow}(c^{\dagger}_{(1,j),\sigma}c_{(2,j),\sigma}+\text{H.c.})\\&-t\sum_{\alpha=1,2}\sum_{j=1}^{N}\sum_{\sigma=\uparrow,\downarrow}(c^{\dagger}_{(\alpha,j),\sigma}c_{(\alpha,j+1),\sigma}+\text{H.c.})\\&+U\sum_{\alpha=1,2}\sum_{j=1}^{N}n_{(\alpha,j),\uparrow}n_{(\alpha,j),\downarrow}\\&+V\sum_{j=1}^{N}\sum_{\sigma,\tau=\uparrow,\downarrow}n_{(1,j),\sigma}n_{(2,j),\tau},\end{aligned} \tag{2}$$

where $t_{\perp}$, t, U, and V are positive parameters, and H.c. represents the Hermitian conjugate. The operators $c^{\dagger}_{x,\sigma}$, $c_{x,\sigma}$, and $n_{x,\sigma}\equiv c^{\dagger}_{x,\sigma}c_{x,\sigma}$ are the creation, the annihilation, and the number operators, respectively, for an electron with spin $\sigma=\uparrow,\downarrow$ at site x. They satisfy the anticommutation relations

$$\{c^{\dagger}_{x,\sigma},c_{y,\tau}\}=\delta_{xy}\delta_{\sigma\tau}, \tag{3}$$

$$\{c^{\dagger}_{x,\sigma},c^{\dagger}_{y,\tau}\}=\{c_{x,\sigma},c_{y,\tau}\}=0. \tag{4}$$

The electron filling factor is defined by $n\equiv N_{\mathrm{e}}/(2|\Lambda|)$, where N_{e} is the number of electrons. The local spin operators are defined by $S^{(\beta)}_x\equiv\frac{1}{2}\Sigma_{\sigma,\tau=\uparrow,\downarrow}c^{\dagger}_{x,\sigma}(p^{(\beta)}_{\sigma\tau})c_{x,\tau}$, where $p^{(\beta)}_{\sigma\tau}$ with $\beta=1,2,3$ are the Pauli matrices. We also define $S^{(\beta)}_{\mathrm{tot}}\equiv\Sigma_{x\in\Lambda}S^{(\beta)}_x$. We denote by $S_{\mathrm{tot}}(S_{\mathrm{tot}}+1)$ the eigenvalue of $(\mathbf{S}_{\mathrm{tot}})^2=\Sigma_{x,y\in\Lambda}\Sigma_{\beta=1}^{3}S^{(\beta)}_xS^{(\beta)}_y$.

The single-electron dispersion relations for the model are given by $\epsilon_{\pm}(k)=-2t\cos k\pm t_{\perp}$ with wave numbers $k=2\pi n/N$ $[n=0,\pm1,\ldots,\pm(N/2-1),N/2]$. The eigenstates with energies $\epsilon_{-}(k)$ and $\epsilon_{+}(k)$ can be written as $b^{\dagger}_k\Phi_0\equiv N^{-1/2}\Sigma_{j=1}^{N}e^{ikj}b^{\dagger}_{j,\sigma}\Phi_0$ and $a^{\dagger}_k\Phi_0\equiv N^{-1/2}\Sigma_{j=1}^{N}e^{ikj}a^{\dagger}_{j,\sigma}\Phi_0$, respectively, where Φ_0 is the no electron state on Λ, and $b^{\dagger}_{j,\sigma}\equiv(c^{\dagger}_{(1,j),\sigma}+c^{\dagger}_{(2,j),\sigma})/\sqrt{2}$, and $a^{\dagger}_{j,\sigma}\equiv(c^{\dagger}_{(1,j),\sigma}-c^{\dagger}_{(2,j),\sigma})/\sqrt{2}$. These operators also satisfy the anticommutation relations.

III. THE CASE OF $U-V\to\infty$ AND $V\to\infty$

In this section, we prove that in the limit $U-V\to\infty$ and $V\to\infty$ the model exhibits saturated ferromagnetism for $N<N_{\mathrm{e}}<2N$. The proof is based on the Perron-Frobenius theorem,[10] which states us that a real symmetric matrix with nonpositive off-diagonal elements satisfying the connectivity condition has a nondegenerate minimum eigenvalue and the corresponding eigenstate which is a linear combination of all basis states with positive coefficients. One can find similar arguments in Refs. 10 and 22. In the following, we first prepare an appropriate basis and then show that the matrix representation of H with respect to this basis satisfies the conditions needed for the Perron-Frobenius theorem.

Since N is even and the periodic boundary conditions are imposed on the model, we assume here that the electron number N_{e} is odd; otherwise the electron hoppings between $(\alpha,1)$ and (α,N) would generate a wrong sign for the Perron-Frobenius theorem.

In the limit $U-V\to\infty$, there is an infinite gap between energies of states with and without doubly occupied sites. In the space without doubly occupied sites, the minimum energy of the interaction terms for $N<N_{\mathrm{e}}<2N$ is $V(N_{\mathrm{e}}-N)$, which is attained by the states with no empty rungs.

Taking account of these, we now prepare a basis for the N_{e}-electron Hilbert space where $H-V(N_{\mathrm{e}}-N)$ has finite energy in the limit $U-V\to\infty$ and $V\to\infty$. Since there are no doubly occupied sites in a finite-energy state for $H-V(N_{\mathrm{e}}-N)$ in this limit, basis states are characterized by position configurations $A\subset\Lambda$ and spin configurations $\sigma_A=\{\sigma_x\}_{x\in A}$, with $\sigma_x=\uparrow,\downarrow$, of electrons. From this together with the restriction that the eigenvalue of interaction terms must be always $V(N_{\mathrm{e}}-N)$, we find it convenient to use the following basis states Φ_{A,σ_A}:

$$\Phi_{A,\sigma_A}=D\prod_{x\in A}c^{\dagger}_{x,\sigma_x}\Phi_0, \tag{5}$$

$$D=\exp\left(i\pi\sum_{\alpha=1,2}\sum_{j=1}^{N/2}\sum_{\sigma=\uparrow,\downarrow}n_{(\alpha,2j),\sigma}\right), \tag{6}$$

where $A\subset\Lambda$ such that $|A|=N_{\mathrm{e}}$ and $A\cap\{(1,j),(2,j)\}\neq\emptyset$ for any j, i.e., A needs to contain at least one site from each rung. Here we use the convention that the product of fermion operators is ordered in such a way that $c^{\dagger}_{(\alpha,j),\sigma_{(\alpha,j)}}$ is always on the left of $c^{\dagger}_{(\alpha',j'),\sigma_{(\alpha',j')}}$ if $j<j'$ or $\alpha<\alpha'$ in the case of $j=j'$. The phase factor D takes 1 if the total number of electrons in $2i$th rungs is even and takes -1 otherwise. This phase factor cancels out an extra minus sign coming from exchanges of fermion operators, when an electron hops in the chain direction. We denote by $\mathcal{P}$ the projection operator onto the space spanned by these basis states.

Let $\widetilde{H}=\mathcal{P}H\mathcal{P}-V(N_{\mathrm{e}}-N)$. Because of the sign convention in Eq. (6) (the total number of electrons in $2i$th rungs varies by exactly one when an electron hops in the chain direction), we have

$$\langle\Phi_{B,\tau_B},\widetilde{H}\Phi_{A,\sigma_A}\rangle=\begin{cases}-t_{\perp} & \text{if}\quad B=A_{(\alpha,j)\to(\alpha',j)}\quad\text{with}\quad|\alpha-\alpha'|=1\\ & \text{and}\quad \tau_B=\overline{\sigma}_{A_{(\alpha,j)\to(\alpha',j)}}\\ -t & \text{if}\quad B=A_{(\alpha,j)\to(\alpha,j')}\quad\text{with}\quad|j-j'|=1\\ & \text{and}\quad \tau_B=\overline{\sigma}_{A_{(\alpha,j)\to(\alpha,j')}}\\ 0 & \text{otherwise,}\end{cases} \tag{7}$$

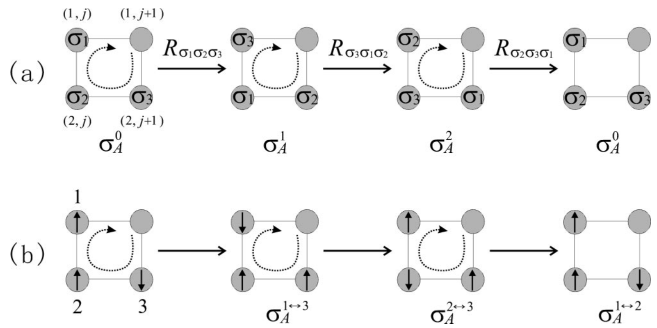

FIG. 2. (a) The spin exchange on a length-4 loop. (b) An example of exchange of spins with $\sigma_1=\uparrow$, $\sigma_2=\uparrow$, and $\sigma_3=\downarrow$.

where $A_{x\to y}$ is defined for A satisfying both $x\in A$ and $y\notin A$ by $A_{x\to y}\equiv(A\setminus\{x\})\cup\{y\}$, which is the position configuration obtained when the electron at site x in A hops to site y. $\overline{\sigma}_{A_{x\to y}}=\{\overline{\sigma}_{x'}\}_{x'\in A_{x\to y}}$ is the spin configuration obtained from σ_A by setting $\overline{\sigma}_y=\sigma_x$ and $\overline{\sigma}_{x'}=\sigma_{x'}$ for $x'\in A\setminus\{x\}$.

Now, we verify the connectivity condition, i.e., for any pair of (A,σ_A) and (B,τ_B) such that $\Sigma_{x\in A}\sigma_x=\Sigma_{x\in B}\tau_x$, there exists integer m such that $\langle\Phi_{B,\tau_B},(\tilde{H})^m\Phi_{A,\sigma_A}\rangle\neq 0$.

We first consider a position configuration A in which there are electrons at $(1,j)$, $(2,j)$, and $(2,j+1)$, and a spin configuration σ_A^0 with $\sigma_{(1,j)}^0=\sigma_1$, $\sigma_{(2,j)}^0=\sigma_2$, and $\sigma_{(2,j+1)}^0=\sigma_3$. Let us define

$$R_{\sigma\tau v}=\mathcal{P}c^\dagger_{(1,j),v}c_{(1,j+1),v}\mathcal{P}c^\dagger_{(2,j),\sigma}c_{(1,j),\sigma}\mathcal{P}\times c^\dagger_{(2,j+1),\tau}c_{(2,j),\tau}\mathcal{P}c^\dagger_{(1,j+1),v}c_{(2,j+1),v}\mathcal{P}. \tag{8}$$

It is easy to see that

$$R_{\sigma_1\sigma_2\sigma_3}\Phi_{A,\sigma_A^0}=\Phi_{A,\sigma_A^1}, \tag{9}$$

where σ_A^1 is the spin configuration obtained from σ_A^0 by setting $\sigma^1_{(1,j)}=\sigma^0_{(2,j+1)}$, $\sigma^1_{(2,j)}=\sigma^0_{(1,j)}$, $\sigma^1_{(2,j+1)}=\sigma^0_{(2,j)}$, and $\sigma^1_{x'}=\sigma^0_x$ for the rest sites $x'\in A$. Similarly we have $R_{\sigma_3\sigma_1\sigma_2}\Phi_{A,\sigma_A^1}=\Phi_{A,\sigma_A^2}$ and $R_{\sigma_2\sigma_3\sigma_1}\Phi_{A,\sigma_A^2}=\Phi_{A,\sigma_A^0}$, where σ_A^2 is determined by using the same procedure as in the case of σ_A^1 [see Fig. 2(a)]. Since the operator $R_{\sigma\tau v}$ is a product of nearest-neighbor hopping terms, and furthermore since possible configurations of $(\sigma_1,\sigma_2,\sigma_3)$ are classified into two patterns: one such that all spins are in the same direction and the other such that the direction of one spin is opposite to that of the other two spins, we find from the above results that $\langle\Phi_{A,\sigma_A^{x\leftrightarrow y}},(\tilde{H})^m\Phi_{A,\sigma_A}\rangle\neq 0$ for some integer m, where $x,y\in\{(1,j),(2,j),(2,j+1)\}$ and $\sigma_A^{x\leftrightarrow y}$ is the spin configuration obtained from σ_A by switching σ_x with σ_y [see Fig. 2(b)].

Next we consider an arbitrary pair of (A,σ_A) and (B,τ_B) such that $\Sigma_{x\in A}\sigma_x=\Sigma_{x\in B}\tau_x$. Let $(\hat{A},\hat{\sigma}_{\hat{A}})$ be the position and spin configurations determined by the following equation:

$$\Phi_{\hat{A},\hat{\sigma}_{\hat{A}}}=\prod_{j;(1,j)\in A\ \text{and}\ (2,j)\notin A}(\mathcal{P}c^\dagger_{(2,j),\sigma_{(1,j)}}c_{(1,j),\sigma_{(1,j)}}\mathcal{P})\times\Phi_{A,\sigma_A}. \tag{10}$$

It is noted that, in the position configuration $\hat{A}$, $N_{\rm e}-N$ sites in chain 1 and all the sites in chain 2 are occupied by electrons because of $N<N_{\rm e}<2N$. Since the right-hand side in Eq. (10) corresponds to successive operations of interchain hopping terms, we find that $\langle\Phi_{\hat{A},\hat{\sigma}_{\hat{A}}},(\tilde{H})^m\Phi_{A,\sigma_A}\rangle\neq 0$ for some integer m. From (i) the comment following (10), (ii) the fact that the electrons in $\hat{A}$ in chain 1 can move in the chain direction, and (iii) the results for the case where the sites $(1,j)$, $(2,j)$, and $(2,j+1)$ are occupied, we conclude that $\langle\Phi_{\hat{B},\hat{\tau}_{\hat{B}}},(\tilde{H})^{m'}\Phi_{\hat{A},\hat{\sigma}_{\hat{A}}}\rangle\neq 0$ for some integer m', where $(\hat{B},\hat{\tau}_{\hat{B}})$ are defined as in the case of $(\hat{A},\hat{\tau}_{\hat{A}})$, and therefore $\langle\Phi_{B,\tau_B},(\tilde{H})^m\Phi_{A,\sigma_A}\rangle\neq 0$ for any pair of (A,σ_A) and (B,τ_B) such that $\Sigma_{x\in A}\sigma_x=\Sigma_{x\in B}\tau_x$ and some integer m. This establishes the connectivity for $\tilde{H}$.

Since we have shown the connectivity and the fact that all the matrix elements of the Hamiltonian in this representation are nonpositive [see Eq. (7)], we can apply the Perron-Frobenius theorem to the Hamiltonian $\tilde{H}$.[5] Therefore, we conclude that the state with the minimum eigenvalue in the subspace of fixed $S_{\rm tot}^{(3)}$ and fixed $N_{\rm e}$ is unique and a linear combination of all basis states (5) with positive coefficients. The ground state in the subspace of $S_{\rm tot}^{(3)}=S_{\rm tot}^{\max}=N_{\rm e}/2$ is nothing but the saturated ferromagnetic ground state. Operating $S_{\rm tot}^-$ to the saturated ferromagnetic state, we can obtain the eigenstates of various subspaces of $S_{\rm tot}^{(3)}$. Because all these states are positive wave functions in the present representation, these states have finite overlap with the states belonging to the minimum eigenvalue in the corresponding subspaces. Therefore, the ground states of $\tilde{H}$ with $N<N_{\rm e}<2N$ in the limit $U-V\to\infty$ and $V\to\infty$ have the total spin $S_{\rm tot}=S_{\rm tot}^{\max}$, and are nondegenerate apart from the trivial $(2S_{\rm tot}^{\max}+1)$-fold degeneracy.

Once we find that the ground states are saturated ferromagnetic, we can obtain their explicit expressions by considering the subspace with $S_{\rm tot}^{(3)}=S_{\rm tot}^{\max}$. The problem we should solve is finding the minimum energy state for the hopping Hamiltonian,

$$\begin{aligned}\tilde{H}_\uparrow&=-t\sum_{\alpha=1,2}\sum_{j=1}^{N}\mathcal{P}(c^\dagger_{(\alpha,j),\uparrow}c_{(\alpha,j+1),\uparrow}+\text{H.c.})\mathcal{P}\\&\quad-t_\perp\sum_{j=1}^{N}\mathcal{P}(c^\dagger_{(1,j),\uparrow}c_{(2,j),\uparrow}+\text{H.c.})\mathcal{P}\\&=-t\sum_{j=1}^{N}\mathcal{P}(a^\dagger_{j,\uparrow}a_{j+1,\uparrow}+b^\dagger_{j,\uparrow}b_{j+1,\uparrow}+\text{H.c.})\mathcal{P}\\&\quad+t_\perp\sum_{j=1}^{N}\mathcal{P}(a^\dagger_{j,\uparrow}a_{j,\uparrow}-b^\dagger_{j,\uparrow}b_{j,\uparrow})\mathcal{P},\end{aligned} \tag{11}$$

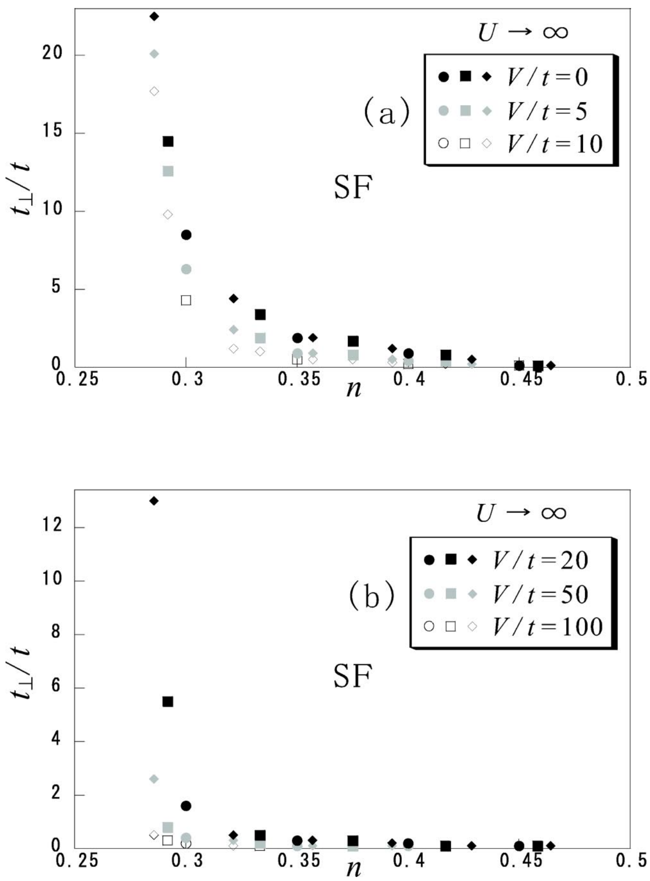

FIG. 3. The critical values of $t_\perp/t$, above which the ground states in the limit $U\to\infty$ have $S_{\rm tot}=N_{\rm e}/2$, as a function of filling factor n for (a) $V/t=0,5,10$, (b) $V/t=20,50,100$. The symbols of circle, square, and diamond represent the data for 10-site, 12-site, and 14-site systems, respectively.

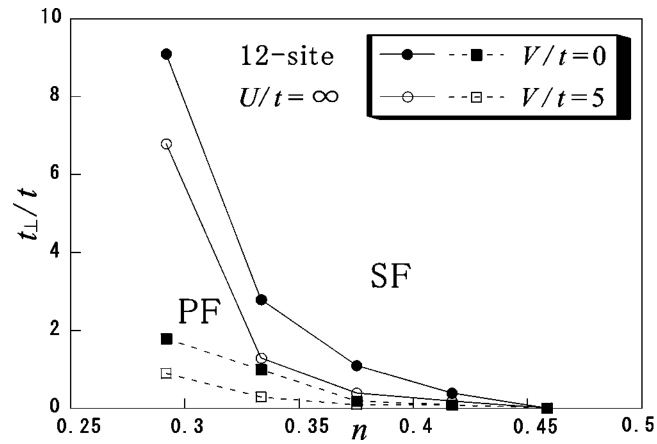

FIG. 4. Magnetic phase diagrams in the limit $U\to\infty$ as a function of filling factor n for 12-site system with $V/t=0,5$. The region indicated by PF between the solid line and the dashed line is the partially polarized ferromagnetic phase.

in this subspace. The operators $a^\dagger_{j,\uparrow}$ ($a_{j,\uparrow}$) and $b^\dagger_{j,\uparrow}$ ($b_{j,\uparrow}$) are those defined in the preceding section. Here let us introduce the following new basis states Ψ_{L_a,L_b}:

$$\Psi_{L_a,L_b}=\left(\prod_{j\in L_a} a_{j,\uparrow}\right)\left(\prod_{j\in L_b} b_{j,\uparrow}\right)\Psi_0, \tag{12}$$

$$\Psi_0=\left(\prod_{j=1}^{N} a^\dagger_{j,\uparrow}\right)\left(\prod_{j=1}^{N} b^\dagger_{j,\uparrow}\right)\Phi_0, \tag{13}$$

where L_a and L_b are arbitrary subsets of $\{1,\ldots,N\}$ such that $|L_a|+|L_b|=2N-N_{\rm e}$ and $L_a\cap L_b=\varnothing$, which comes from the original condition $A\cap\{(1,j),(2,j)\}\neq\varnothing$ for all j mentioned below Eq. (6). We rewrite $\tilde{H}_\uparrow$ as

$$\tilde{H}_\uparrow=t\sum_{j=1}^{N}\mathcal{P}(a_{j+1,\uparrow}a^\dagger_{j,\uparrow}+b_{j+1,\uparrow}b^\dagger_{j,\uparrow}+\text{H.c.})\mathcal{P}$$
$$-t_\perp\sum_{j=1}^{N}\mathcal{P}(a_{j,\uparrow}a^\dagger_{j,\uparrow}-b_{j,\uparrow}b^\dagger_{j,\uparrow})\mathcal{P}, \tag{14}$$

and regard $a_{j,\uparrow}$ ($a^\dagger_{j,\uparrow}$) and $b_{j,\uparrow}$ ($b^\dagger_{j,\uparrow}$) as annihilation (creation) operators of "an up-spin electron" and "a down-spin electron," respectively. Then by taking into account the condition $L_a\cap L_b=\varnothing$ on the new basis states, we find that the system is equivalent to the Hubbard model with infinite on-site repulsion on the length-N periodic linear chain in the magnetic field $t_\perp$. From this correspondence, we find that the minimum energy state of $\tilde{H}_\uparrow$ in the subspace with $S^{(3)}_{\rm tot}=S^{\rm max}_{\rm tot}$ is given by

$$\Phi_{\rm ferro}=\left(\prod_{k;|k|>\pi(N_{\rm e}-N-1)/N} a_{k,\uparrow}\right)\Psi_0$$
$$=\left(\prod_{k;|k|\leq\pi(N_{\rm e}-N-1)/N} a^\dagger_{k,\uparrow}\right)\left(\prod_{\text{all }k} b^\dagger_{k,\uparrow}\right)\Phi_0. \tag{15}$$

Therefore $\Phi_{\rm ferro}$ and its SU(2) rotations are the ground states of $\tilde{H}$. These ground states allow gapless charge excitations, so that our model exhibits metallic ferromagnetism.

It is noted that for $N_{\rm e}=2N-1$ in the limit $U\to\infty$ the model exhibits saturated ferromagnetism (Nagaoka's ferromagnetism) for any V.

IV. THE RESULTS OF NUMERICAL CALCULATIONS

In this section, we investigate the ground-state magnetic properties of the model with $N<N_{\rm e}<2N$ for finite U and V by numerical calculations based on the Lanczos method. The argument in the preceding section holds also for the model with open boundary conditions, in which case we can remove the restriction of $N_{\rm e}$ being odd and prove the occurrence of ferromagnetism for any integer $N_{\rm e}$ in $N<N_{\rm e}<2N$. Taking account of this fact, we have performed the numerical calculations by adopting the open boundary conditions, except for the results shown in Fig. 4.

First, we examine the effect of V on ferromagnetism in the limit $U\to\infty$. In Fig. 3, we plot the critical values $t_{\perp c}/t$, above which the ground states are saturated ferromagnetic (SF), as a function of n for (a) $V/t=0,5,10$, and (b) $V/t=20,50,100$. Although calculations are performed on small systems, one can see that the data in the various lattice sizes are scaled to a single line, which indicates that the finite-size effect is small. The result for $V/t=0$ is consistent with

Kohno's result.[22] Figure 3 shows that, as V/t increases, the saturated ferromagnetic ground states can exist for almost all positive values of $t_\perp/t$ over the range of $1/4<n<1/2$, which is consistent with the result in the preceding section. By using DMRG, Liang and Pang determined the critical electron density $n_c \simeq 0.39$, below which saturated ferromagnetism is unstable, for $t_\perp/t=1$ in the absence of V.[24] The present results indicate that n_c decreases when V is introduced.

Next, Fig. 4 is the magnetic phase diagrams on the $(t_\perp/t,n)$ plane for $V=0,5$. The ground states are partially polarized ferromagnetic in the region indicated by PF. Since PF phase boundaries could not be accurately determined with open boundary conditions, we carried out the calculations by taking other boundary conditions; here we imposed periodic boundary conditions for $N_e=7,9,11$ and antiperiodic boundary conditions for $N_e=8,10$ on the 12-site system.[25] Figure 4 shows that PF phase as well as SF phase extends to lower values of $t_\perp/t$ by V/t.

Finally, we show the critical values U_c/t above which the ground states are SF. In Fig. 5, we show the critical values U_c/t as a function of n with V/t varied from 0 to 10 for (a) $t_\perp/t=1$, (b) $t_\perp/t=2$, and (c) $t_\perp/t=5$. When V/t is introduced, U_c/t are greatly reduced on the 1/4-filling side, particularly for small $t_\perp/t$, although there are almost no changes in U_c/t on the 1/2-filling side. These results indicate that the effect of V/t on ferromagnetism is important for low filling and small $t_\perp/t$. In Fig. 6, we show the result of U_c/t for $V/t=100$. Figure 6 indicates that SF states remain stable even for exceedingly large V/t provided $U>V$. To confirm whether the effect of V/t is large on the 1/4-filling side for small $t_\perp/t$, we have calculated U_c/t as a function of V/t for 12-site systems with $t_\perp/t=2$. We show the results for (a) $N_e=8$ ($n\sim 0.333$), $N_e=9$ ($n=0.375$), and (b) $N_e=10$ ($n\sim 0.417$), $N_e=11$ ($n\sim 0.458$) in Fig. 7, which clearly indicate that U_c/t on the 1/4-filling side (a) is dramatically reduced due to V/t, while there is almost no influence of V/t on U_c/t on the 1/2-filling side (b). Figure 8 is the SF phase diagram on the $(U/t,t'/t)$ plane for $N_e=9$ with $V/t=0,5$. We find that SF region clearly extends to small $t_\perp/t(\leqslant 3)$ due to V/t.

Kohno's result with $V=0$ for $1/4<n<1/2$ in the limit $U\to\infty$ shows that sufficiently large $t_\perp/t$ makes the ground state to be saturated ferromagnetic.[22] For sufficiently large $t_\perp/t$, the band gap $2t_\perp-4t$ between the lower single-electron band and the upper single-electron band is sufficiently large. In this case the ground state is obtained by filling up the low single-electron energy levels by up-spin electrons; namely, the lower band corresponding to $b_{k,\sigma}^\dagger\Phi_0$ is completely filled by up-spin electrons and the upper band corresponding to $a_{k,\sigma}^\dagger\Phi_0$ is partially occupied by the other up-spin electrons. This state is just equal to the state (15). When V is switched on, in the limit of $U-V\to\infty$ and $V\to\infty$, our rigorous proof shows the existence of saturated ferromagnetism for finite $t_\perp/t$ not restricted to sufficiently large $t_\perp/t$ in contrast with Kohno's model. Furthermore, it should be noted that when V/t is sufficiently large the state (15) remains as the ground state for small values of $t_\perp/t$, even where the energy gap between upper and lower bands

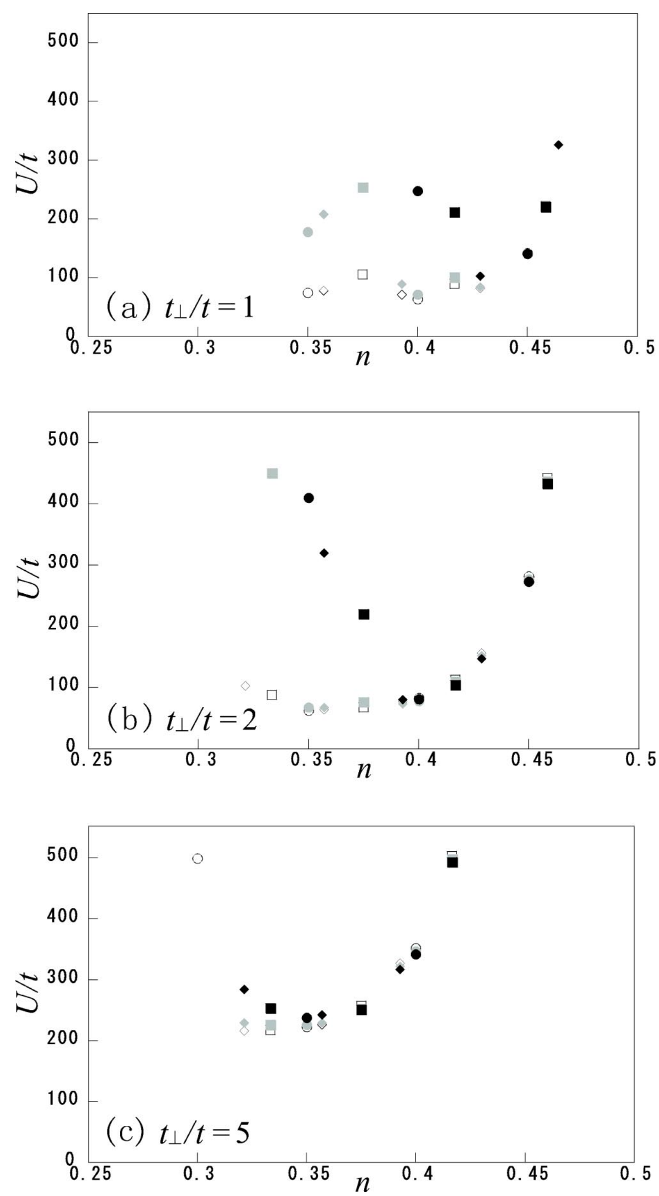

FIG. 5. The critical values of U/t, above which the ground states are SF, as a function of filling factor n for (a) $t_\perp/t=1$, (b) $t_\perp/t=2$, and (c) $t_\perp/t=5$. The black, gray, and white symbols denote the results for $V/t=0,5$, and 10, respectively. The symbols of circle, square, and diamond represent the data for 10-site, 12-site, and 14-site systems, respectively.

disappears. This ground state is different from the state obtained by filling up the low single-electron energy levels by up-spin electrons. Our numerical calculations in the limit $U\to\infty$ show that the critical value $t_{\perp c}/t$ decreases with the increase of V/t. Thus, the off-site repulsion V/t seems to increase $t_\perp/t$ effectively or compensate the role of $t_\perp/t$. Moreover, our results for finite U/t show that the introduction of V/t dramatically reduces U_c/t for small $t_\perp/t$, and that the effect of V/t in the limit $U\to\infty$ persists also in the case of finite U/t. In the absence of V, the sufficiently large band gap induces ferromagnetism, while U_c/t increases as the band gap increases [see Fig. 5(c)]. On the other hand, sufficiently large V/t can realize the state (15) as the ground

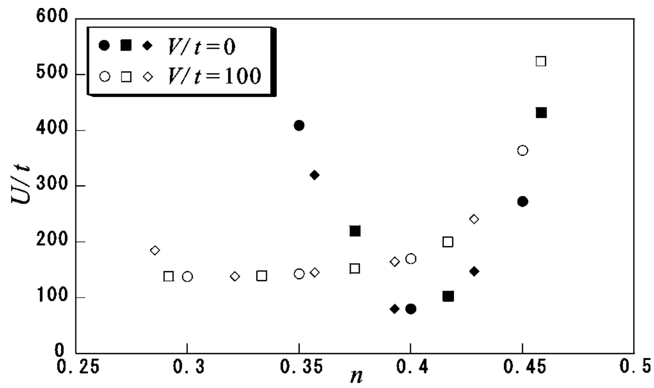

FIG. 6. The critical values of U/t as a function of filling factor n for $t_{\perp}/t=2$. The black and white symbols denote the results for $V/t=0$ and 100, respectively. The symbols of circle, square, and diamond represent the data for 10-site, 12-site, and 14-site systems, respectively.

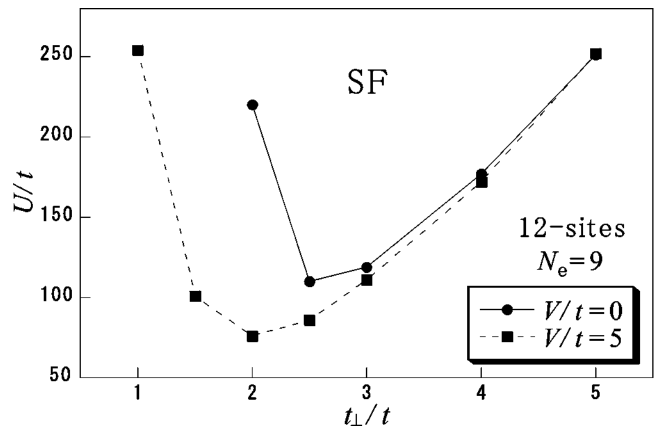

FIG. 8. The critical values U_c/t as a function of $t_{\perp}/t$ for $N_e=9$ and 12-site system. The symbols of circle and square represent the data for $V/t=0$ and 5, respectively.

state even if the band gap is small or absent. Thus U_c/t decreases for small $t_{\perp}/t$.

V. SUMMARY AND DISCUSSION

To summarize, in the extended Hubbard model with the interchain off-site repulsion V on the two-leg ladder, we rigorously proved that the ground states are saturated ferromagnetic for $1/4<n<1/2$ in the limit $U-V\to\infty$ and $V\to\infty$. We also gave an example of the fully polarized metallic ground states for the extended Hubbard model. As far as we know, this is the first time that the exact expression of the ferromagnetic ground states for the extended Hubbard model with the off-site repulsion is obtained. By using numerical calculations, we found the region where $t_{\perp c}/t$ is reduced in the magnetic phase diagrams when V is introduced in the limit $U\to\infty$. Furthermore, we showed that U_c/t is reduced due to V, particularly on the 1/4-filling side for small $t_{\perp}/t$.

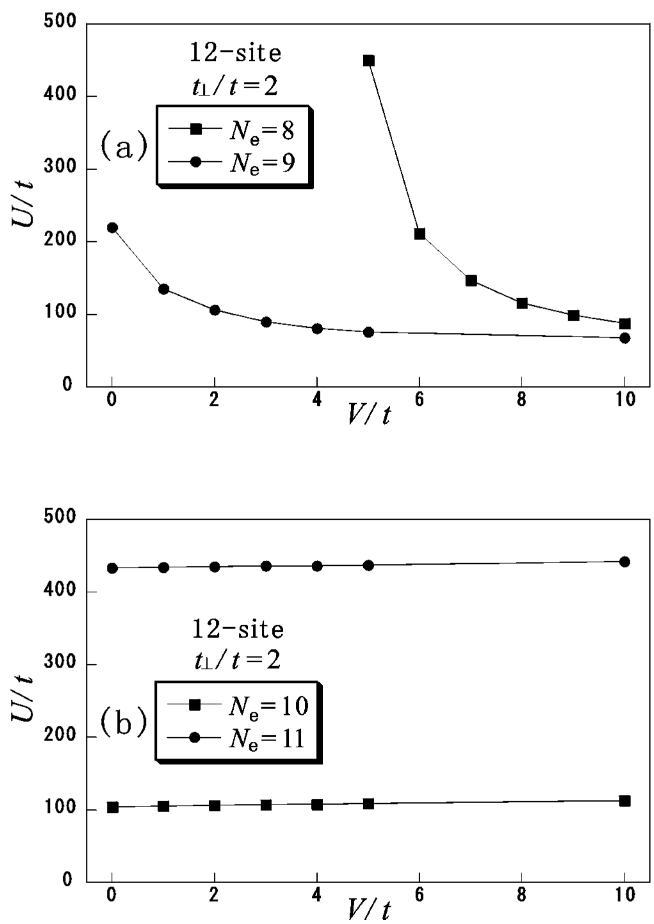

FIG. 7. The critical values of U/t as a function of V/t for $t_{\perp}/t=2$ and 12-site system. These are the results for (a) $N_e=8,9$ and (b) $N_e=10,11$, respectively.

In this paper, we concentrate our attention on the case where the intrachain off-site repulsion $V_{\parallel}$ is absent, but generally its effects should be considered. We first note that the proof in Sec. III, which is based on the Perron-Frobenius theorem, is applicable to the model including $V_{\parallel}$ and such model is proved to exhibit saturated ferromagnetism in the limit $U-V\to\infty$ and $V\to\infty$ if $|V_{\parallel}|<\infty$. In this case, however, the state (15) is no longer the exact ground state of this model. On the other hand, Vojta *et al.* showed that, in the case $V_{\parallel}=V_{\perp}=V$, the incommensurate spin correlations tend to be enhanced near 1/4 filling and suppressed near 1/2 filling as V increases.[23] From these results, it is expected that the anisotropy of off-site repulsion plays an important role in stabilization of ferromagnetism, and it is an interesting future problem to investigate whether similar effects will be observed in models with anisotropic off-site repulsion on other lattices.

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