Ferromagnetism in the strong-coupling regime of the one-dimensional Kondo-lattice model

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The ground state of the one-dimensional Kondo lattice model is examined in the strong-coupling regime. An effective Hamiltonian is developed to describe low-energy processes. This leads to a ferromagnetic ground state in this regime for all conduction electron densities. The spin excitations are those of a squeezed spin chain with ferromagnetic Heisenberg exchange coupling. In addition there are quasiparticle excitations, which are discussed in detail only for the case of half filling.

I. INTRODUCTION

The ground-state properties of various strongly correlated electron systems is a very actively discussed topic at present. One reason for this development is the discovery of the class of heavy fermion materials. The standard models for the description of heavy fermion systems is the Kondo lattice model (KLM) or the more fundamental periodic Anderson model (PAM).[1]

In this paper the one-dimensional (1D) KLM is discussed. It consists of a lattice of localized spins $\{S_j\}$ interacting with otherwise free conduction electrons via a local spin-exchange interaction. The corresponding Hamiltonian has the well-known form

$$H=-t\sum_{\langle i,j\rangle}\sum_{s}c_{is}^{\dagger}c_{js}+\text{H.c.}-J\sum_{i}\mathbf{S}_i\cdot\mathbf{s}_i\ , \tag{1}$$

where

$$S_l^{\mu}=\frac{1}{2}\sum_{s,s'}f_{is}^{\dagger}\sigma_{ss'}^{\mu}f_{is'}\ ,\quad s_l^{\mu}=\frac{1}{2}\sum_{s,s'}c_{is}^{\dagger}\sigma_{ss'}^{\mu}c_{is'}\ . \tag{2}$$

The operators $c_{is}^{\dagger}(c_{is})$ and $f_{is}^{\dagger}(f_{is})$ denote the conduction electron and localized electron operators, respectively. Since charge fluctuations are not allowed for the localized electrons, the f operator satisfies the operator identity, $f_{i\uparrow}^{\dagger}f_{i\uparrow}+f_{i\downarrow}^{\dagger}f_{i\downarrow}=1$ for all sites i. For simplicity, we assume that the hopping term connects only nearest-neighbor sites i and j. The exchange-coupling constant is chosen to be negative leading to antiferromagnetic coupling between the localized and conduction electron spins, $\mathbf{S}_i$ and $\mathbf{s}_i$.

Various methods have been developed to treat this system. Techniques, like the $1/N_f$ expansion (N_f is the degeneracy of the localized orbitals in the PAM or the localized spins in the KLM),[2] slave-boson methods,[3] or variational treatments by Gutzwiller wave functions,[4,5] have been successful in explaining various properties of these systems, e.g., the formation of a coherent band of quasiparticles with a heavy effective mass. However, these methods are not sufficient to determine the symmetry of the ground state definitely.

Information about the ground-state symmetry is obtained by both quantum Monte Carlo[6] and exact diagonalization[7,8] which provide a bulk of significant results on the 1D KLM and PAM. However, there are clear limitations in these numerical studies due to the smallness of the tractable systems and the restriction to one dimension.

Rigorous statements about the ground state are available only for some limiting cases yielding, however, reliable tests for approximate treatments. It can be proved that the half-filled (symmetric) PAM has a spin singlet ground state in any dimension, implying a similar result for the KLM.[9] On the other hand, in the limit of vanishing carrier concentration one can show rigorously that the ground state of the KLM is ferromagnetic (with incompletely saturated magnetization).[10,11]

Various attempts have been undertaken to clarify the ground-state phase diagram of both the KLM and the PAM.[12,13] Recently, Fazekas and Müller-Hartmann gave an extensive discussion of the phase diagram in the n_c-J plane (n_c is the conduction electron density) for the KLM in 1D and 2D. They obtain the phase diagram by comparing the energies of several variational states using Gutzwiller wave functions for a (Kondo) singlet state and mean-field wave functions for various magnetically ordered states.[13] Their result for the 1D system states that

in the weak-coupling limit a region of ferromagnetic order appears for small n_c which evolves into a state with spiral spin correlation as n_c is increased. In the strong-coupling regime the ground state forms a singlet which describes the heavy fermion state.

Recently, Troyer and Würtz[14] performed quantum Monte Carlo calculations of the 1D KLM at intermediate electron concentrations and found that the ferromagnetic ground state occupies a far wider region of the phase diagram than obtained by Fazekas and Müller-Hartmann.[13] In this paper we will prove that the ground state is ferromagnetic for all electron concentrations $n_c(\neq 1)$ in the strong-coupling limit of the 1D KLM.

II. THE EFFECTIVE HAMILTONIAN IN THE STRONG-COUPLING LIMIT

In the infinitely strong-coupling case ($J=-\infty$) the conduction electrons form an on-site spin-singlet configuration together with the localized spin of the same site. The nearest-neighbor transfer of the conduction electrons allows these on-site singlet pairs (OSSP) to move accompanied with a backflow of localized spins, just like the motion of holes in the $U-\infty$ Hubbard model. In the 1D system this leads to the peculiar situation that the available spin degrees of freedom are degenerate. Like in the 1D $U=\infty$ Hubbard model only the charge but not the spin configuration can be changed through the motion of an OSSP. A partial lifting of the complete spin degeneracy occurs through cyclic permutation if the chain forms a closed ring of finite length with periodic, antiperiodic, or twisted boundary condition.[15] (This point is considered also briefly in Sec. IV). We will, however, neglect this point and consider the spin degeneracy to be complete as it would be for open chains or infinite systems. Then the question arises which spin configuration would be favored, if we take into account the first-order corrections in a t/J expansion around the infinite coupling point. Introducing a new effective Hamiltonian to describe the strong-coupling limit, we can show that this ground state is ferromagnetic, polarizing all unpaired localized spins.

To obtain this effective Hamiltonian we integrate out the virtual processes which yield configurations containing an on-site spin triplet pair (OSTP) or a site occupied by two conduction electrons with a cost in exchange energy of $|J|$ and $3|J|/2$, respectively. The resulting Hamiltonian operates in a reduced Hilbert space which contains only sites occupied by an OSSP or by a single localized spin (for a detailed derivation see the Appendix).

Introducing the new creation (annihilation) operators $\tilde{f}_{is}^{\dagger}=(1-n_{ci})f_{is}^{\dagger}$ [$\tilde{f}_{is}=(1-n_{ci})f_{is}$] with $n_{ci}=\sum_s c_{is}^{\dagger}c_{is}$ we can write this Hamiltonian as

$$\tilde{H}=\sum_{l=1}^{5} H_l \tag{3}$$

with

$$H_1=-\frac{t}{2}\sum_{i,s}(\tilde{f}_{i+1,s}^{\dagger}\tilde{f}_{is}+\text{H.c.})+\frac{3J}{4}\sum_i(1-\tilde{n}_i)\ ,$$

$$H_2=-\frac{t^2}{2J}\sum_{i,s}(\tilde{f}_{i+1,s}^{\dagger}\tilde{n}_i\tilde{f}_{i-1,s}+\text{H.c.})\ ,$$

$$H_3=+\frac{t^2}{4J}\sum_{i,s,s'}(\tilde{f}_{i+1,s'}\tilde{f}_{i,s}^{\dagger}\tilde{f}_{i,s'}\tilde{f}_{i-1,s}+\text{H.c.})\ ,$$

$$H_4=-\frac{t^2}{6J}\sum_{i,s}[\tilde{f}_{i+1,s}^{\dagger}(1-\tilde{n}_i)\tilde{f}_{i-1,s}+\text{H.c.}]\ ,$$

$$H_5=-\frac{5t^2}{6J}\sum_i\tilde{n}_{i+1}\tilde{n}_i+\frac{t^2}{6J}\sum_i(\tilde{n}_i+4)\ ,$$

where $\tilde{n}_i=\sum_s\tilde{f}_{is}^{\dagger}\tilde{f}_{is}$, L is the system size, and the $\tilde{f}$ operators are restricted to $\tilde{f}_{i\uparrow}^{\dagger}\tilde{f}_{i\uparrow}\tilde{f}_{i\downarrow}^{\dagger}\tilde{f}_{i\downarrow}=0$ for all sites, i.e., no double occupancy of $\tilde{f}$ states is allowed. In this Hamiltonian the half-filled Kondo lattice corresponds to the system with no $\tilde{f}$ electrons, i.e., the $\tilde{f}$-electron vacuum. If all sites are occupied by one $\tilde{f}$ electron the original KLM contains no conduction electrons, again yielding complete spin degeneracy.

The part H_1 of the effective Hamiltonian contains the contributions of the order t and J, the nearest-neighbor hopping and the chemical potential. If we restrict ourselves to H_1 the charge and spin degrees of freedom are decoupled in the Hilbert space. The wave function factorizes into charge and spin part as shown by Ogata and Shiba for the $U=\infty$ Hubbard model.[16] This feature is very important for our treatment below.

Introducing now corrections of the order t/J we obtain a series of new processes. The *three site terms* in H_2, H_3, and H_4 describe next-nearest-neighbor hopping processes by overhopping an $\tilde{f}$ electron on the intermediate site with and without spin flip given by H_3 and H_2, respectively, and by overhopping an empty intermediate site in H_4. Among these terms H_2 is the only one which changes the spin configuration. The terms in H_5 represent a repulsive interaction between $\tilde{f}$ electrons on nearest-neighbor sites and a t/J correction of the chemical potential. In this form the Hamiltonian corresponds essentially to the $U=\infty$ Hubbard model including the three-site and the nearest-neighbor interaction terms.

III. LIFTING OF SPIN DEGENERACY

In this section we analyze the symmetry of the ground state when the spin degeneracy of H_1 is lifted by the terms of the order t/J.

A. Rigorous statement

In the leading order of t/J it is possible to prove that the ground state of $\tilde{H}$ is ferromagnetic for any concentration of $\tilde{f}$ electrons. In this order we can use the property of the Hamiltonian H_1 that the wave function can be written in the product form

$$|\Psi\rangle=\sum_{i_1,\ldots,i_N}\sum_{s_1,\ldots,s_N}\Gamma_{i_1,\ldots,i_N}\gamma_{s_1,\ldots,s_N}|i_1,\ldots,i_N\rangle\otimes|s_1,\ldots,s_N\rangle\ , \tag{4}$$

where $|i_1,\ldots,i_N\rangle$ and $|s_1,\ldots,s_N\rangle$ represent basis states of the charge and spin configurations for N $\tilde{f}$-electrons.

The eigenstates $|n\rangle$ of the charge part which are independent of the spin configuration can be given by

$$|\Psi_n(s_1,\ldots,s_N)\rangle = |n\rangle \otimes |s_1,\ldots,s_N\rangle = \sum_{i_1<i_2<\cdots<i_N} \Gamma^{(n)}_{i_1,i_2,\ldots,i_N} \tilde{f}^{\dagger}_{i_1,s_1}\tilde{f}^{\dagger}_{i_2,s_2}\cdots\tilde{f}^{\dagger}_{i_N,s_N}|\text{vac}\rangle \ , \tag{5}$$

where $|\text{vac}\rangle$ denotes the $\tilde{f}$-electron vacuum and N is the number of $\tilde{f}$ electrons (free spins). The wave function $\Gamma^{(n)}_{i_1,i_2,\ldots,i_N}$ can be represented by a Slater determinant for the charge degrees of freedom only.

We analyze now the lifting of the spin degeneracy by means of first-order perturbation for the ground states $\{|0\rangle\otimes|s_1,s_2,\ldots,s_N\rangle\}$ where we take the spin configuration to label the different degenerate states, in short notation, $|s_1,s_2,\ldots,s_N\rangle$. Then the Hamiltonian matrix is given by

$$\langle s_1,s_2,\ldots,s_N|\tilde{H}|s_1',s_2',\ldots,s_N'\rangle = \langle \Psi_0(s_1,s_2,\ldots,s_N)|\tilde{H}|\Psi_0(s_1',s_2',\ldots,s_N')\rangle \ . \tag{6}$$

Apart from H_2, all other terms in $\tilde{H}$ lead to diagonal elements of this matrix and are, for the moment, not of interest for us. The off-diagonal terms have the form

$$\begin{aligned}
&\langle s_1,\ldots,s_{j+1},s_j,\ldots,s_N|H_2|s_1,\ldots,s_j,s_{j+1},\ldots,s_N\rangle \\
&\quad = \left\langle 0\left|\left(-\frac{t^2}{2J}\right)\sum_{i_j}(\tilde{f}^{\dagger}_{i_{j+1},s_j}\tilde{f}^{\dagger}_{i_j,s_{j+1}}f^{\dagger}_{i_j,s_{j+1}}\tilde{f}_{i_j-1,s_j}+\text{H.c.})\right|0\right\rangle \\
&\quad = \frac{t^2}{2J}\left[\sum_{\substack{i_1<\cdots<i_{j-1}<i_j,\\ i_{j+2}<i_{j+2}<\cdots<i_N}} \Gamma^{(0)*}_{i_1,\ldots,i_{j-1},i_j+1,i_j+2,i_{j+2},\ldots,i_N}\Gamma^{(0)}_{i_1,\ldots,i_{j-1},i_j,i_j+1,i_{j+2},\ldots,i_N}\right. \\
&\qquad \left. + \sum_{\substack{i_1<\cdots<i_{j-1}<i_j-2,\\ i_j<i_{j+2}<\cdots<i_N}} \Gamma^{(0)*}_{i_1,\ldots,i_{j-1},i_j-2,i_j-1i_{j+2},\ldots,i_N}\Gamma^{(0)}_{i_1,\ldots,i_{j-1},i_j-1,i_j,i_{j+2},\ldots,i_N}\right]
\end{aligned} \tag{7}$$

for any j between 1 and $N-1$. We claim now that all these off-diagonal matrix elements are negative ($J<0$). To show this we first return to the Hamiltonian H_1 describing the charge degrees of freedom only. In the real-space basis all off-diagonal matrix elements of the corresponding Hamiltonian matrix are nonpositive ($-t<0$). A straightforward application of the Perron-Frobenius theorem leads to the well-known result that the state with lowest energy of this Hamiltonian has a strictly positive (nodeless) wave function in the real space basis ($\Gamma^{(0)}_{i_1,\ldots,i_N}>0$ for all $i_1<\cdots<i_N$ apart from a global gauge). This ground state is unique since the Hamiltonian matrix in real-space representation is completely connected, i.e., any charge configuration can be obtained starting from an arbitrary configuration by successive application of the Hamiltonian (for the Perron-Frobenius theorem see, for example, Ref. 17). This property confirms that the sums in Eq. (7) are strictly positive giving together with the prefactor $t^2/2J$ strictly negative matrix elements.

Thus, the Hamiltonian matrix of Eq. (6) also has no positive off-diagonal elements. This fact allows the application of the Perron-Frobenius theorem to this matrix too. Since the off-diagonal elements correspond each to an exchange (transposition) of two neighboring spins in the spin configuration, all permutations of spins can be reached by successive operation of the Hamiltonian. Hence, this Hamiltonian is completely connected if we restrict to a subspace with fixed S^z_{tot}. Since the Hamiltonian is obviously rotationally invariant in spin space the ground state has definite spin quantum numbers S^2_{tot} and S^z_{tot}. As a result the state with lowest energy is unique and has a strictly positive wave function in the spin-configuration Hilbert space.

In each Hilbert subspace with fixed S^z_{tot} the spin state with maximal S^2_{tot} has one representative with a wave function which is constant in the spin configuration basis. Thus this state has a finite overlap with the ground state in this subspace. Consequently, the ground state of the Hamiltonian matrix [Eq. (6)] is ferromagnetic with the largest possible total spin, $S_{\text{tot}}=N/2$, leading to the following statement:

The spin degeneracy of 1D KLM at $J=-\infty$ is lifted in a perturbative sense towards a ferromagnetic state for *any concentration* n_c of conduction electrons with a *total* spin per site $(1-n_c)/2$.

This statement is valid for sufficiently small values of $|t/J|$. For $|t/J|$ of the order one, however, corrections not taken into account in the proof will be important. Especially, H_3 and H_4 introduce frustrations which become obvious by noticing that they act on the charge configurations leading to off-diagonal matrix elements of $\tilde{H}$ in the complete Hilbert space with their sign opposite to the ones originating from H_2. The Perron-Frobenius theorem cannot be applied in this case. Eventually, these frustrations lead to a qualitative change of the ground-state properties when $|t/J|$ grows to the order of one. This behavior is observed in numerical calculations for finite-size systems which will be discussed elsewhere.

B. The effective spin Hamiltonian

This subsection is devoted to the derivation of the Hamiltonian in the truncated Hilbert space containing

only the spin degrees of freedom. This Hamiltonian has the structure of a Heisenberg model for a spin chain squeezed to the length N compared with the original chain with L lattice sites.

$$H_{\text{spin}}=\sum_{j=1}^{N}(\epsilon-J_{\text{eff}}S_jS_{j+1}) , \tag{8}$$

where we assume periodic boundary conditions, i.e., $S_{N+1}=S_1$. The exchange coupling J_{eff} is isotropic, since the system has the complete rotational symmetry in spin space. The constant ϵ is a spin configuration independent energy shift.

We will now derive J_{eff} and ϵ from the Hamiltonian matrix in Eq. (6). Note that a similar treatment was given by Shiba and Ogata for the 1D t-J model.[16] First, let us define the wave function of the system with infinite coupling. As mentioned above they can be written as Slater determinants.

$$\Gamma^{\{k_i\}}_{i_1,\ldots,i_N}=\text{Det}\begin{bmatrix}\phi_1(i_1) & \cdots & \phi_1(i_N)\\ \vdots & & \vdots\\ \phi_N(i_1) & \cdots & \phi_N(i_N)\end{bmatrix} , \tag{9}$$

where $i_1<i_2<\cdots<i_N$ and $\phi_l(i_j)$ is a one-particle wave function with the moment k_l satisfying the boundary conditions. Since in the infinite system the boundary condition is irrelevant we choose here for convenience the periodic boundary condition, keeping in mind the problem mentioned earlier and in Ref. 15. Thus

$$\phi_l(i_j)=\frac{1}{\sqrt{L}}e^{ik_li_j} \tag{10}$$

with $k_l=2\pi l/L$ with l an integer $-L/2\le l\le L/2-1$ (L is the system size).

The exchange coupling is obtained from the off-diagonal matrix element M_{od} [Eq. (7)], via the relation

$$M_{\text{od}}=\langle s_1,\ldots,s_{j+1},s_j,\ldots,s_N|-J_{\text{eff}}(S_j^+S_{j+1}^-+S_j^-S_{j+1}^+)/2|s_1,\ldots,s_j,s_{j+1},\ldots,s_n\rangle .$$

In the calculation of this off-diagonal matrix element a difficulty occurs by fixing j, i.e., calculating the matrix element for the exchange of the jth and the $(j+1)$th spin. However, if we average over all j the calculation is actually rather simple,[18]

$$M_{\text{od}}=\frac{-t^2}{2J}\frac{1}{N}\sum_{j=1}^{N}\langle 0|\sum_{i_j}(\tilde{f}^\dagger_{i_{j+1},s_{j+1}}\tilde{f}^\dagger_{i_j,s_j}\tilde{f}_{i_j,s_j}\tilde{f}_{i_{j-1},s_{j+1}}+\tilde{f}^\dagger_{i_{j-1},s_{j+1}}\tilde{f}^\dagger_{i_j,s_j}\tilde{f}_{i_j,s_j}\tilde{f}_{i_{j+1},s_{j+1}})|0\rangle . \tag{11}$$

It is convenient to change now from the real to the momentum representation ($\tilde{f}^\dagger_k=\sum_i\phi_k(i)\tilde{f}^\dagger_i$) resulting into the form

$$M_{\text{od}}=\frac{-t^2}{J}\frac{1}{NL^2}\sum_{k\neq k'}\bar{n}_k\bar{n}_{k'}[\cos(2k)-\cos(k+k')] , \tag{12}$$

where $\bar{n}_k$ is the ground-state momentum distribution function, $\bar{n}_k=\theta(\tilde{k}_F-|k|)$ with θ as the step function. The Fermi momentum $\tilde{k}_F$ of the $\tilde{f}$ electrons is given by $\tilde{k}_F=\pi(N-1)/L$, i.e., the Fermi momentum for spinless Fermions. In the limit of infinite L, fixing the density $\rho=N/L$, we obtain

$$M_{\text{od}}=\frac{t^2}{2\pi J}\left[\frac{2}{\pi\rho}\sin^2(\pi\rho)-\sin(2\pi\rho)\right] . \tag{13}$$

Note that $1-\rho$ corresponds to the density of conduction electrons, n_c, in the original KLM.

Thus, J_{eff} as a function of the $\tilde{f}$-electron density is now given by $J_{\text{eff}}(\rho)=-2M_{\text{od}}(\rho)$ as plotted in Fig. 1. The effective exchange coupling J_{eff} is positive so that the ground state exhibits ferromagnetic order as expected from the previous subsection. In the limiting case of half filling for the conduction electrons ($n_c\to 1$, $\rho\to 0$) the effective interaction behaves as $J_{\text{eff}}\to(2t^2/3J)\pi^2\rho^3$ and in the low concentration limit ($\rho\to 1$), $J_{\text{eff}}\to(4\pi t^2/J)(1-\rho)$.

The constant ϵ is obtained from the diagonal part of the Hamiltonian matrix [Eq. (7)], which is obtained in the same way as M_{od}.

$$\frac{M_d}{N}=-\frac{t}{\pi\rho}\sin(\pi\rho)+\frac{3}{4\rho}J+\frac{t^2}{\pi J}\left[\frac{1}{12}\left[\frac{2}{\pi\rho}\sin^2(\pi\rho)-\sin(2\pi\rho)\right]-\frac{1}{6}\frac{\sin(2\pi\rho)}{\rho}+\frac{\pi}{6}-\frac{5\pi}{6}\left[\rho-\frac{1}{\pi^2\rho}\sin^2(\pi\rho)\right]\frac{2\pi}{3\rho}\right] , \tag{14}$$

which is the diagonal matrix element per spin in the system leading to $\epsilon(\rho)=M_d(\rho)/N$.

The ground-state energy per lattice site for the fully spin-polarized state is obtained immediately,

$$E(\rho)=\rho\left[\epsilon(\rho)+\frac{J_{\text{eff}}(\rho)}{4}\right] . \tag{15}$$

In Fig. 2 we plot the corrections in the order t/J to the ground-state energy of H_1. In the limit $\rho\to 0$ (half filling of the KLM) the ground-state energy goes continuously to the value $3J/4+2t^2/3J$ per lattice site. On each site there is one OSSP with the binding energy $3J/4$ for the singlet formation and its polarization energy $2t^2/3J$.

Using the expression for the energy $E(\rho)$, it is easy to calculate the compressibility of the system $\kappa^{-1}=\rho^2\partial^2E(\rho)/\partial\rho^2$,

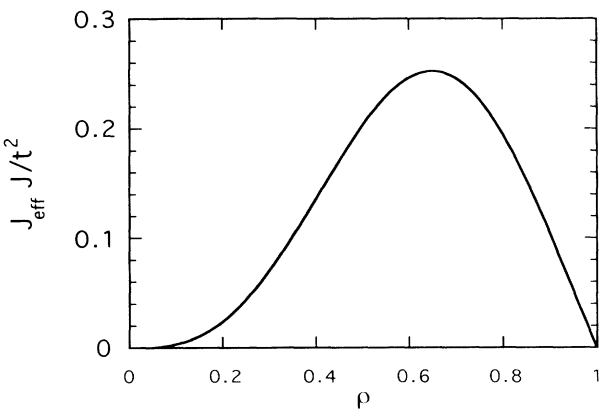

FIG. 1. Effective spin-exchange coupling as function of the $\tilde{f}$-electron concentration.

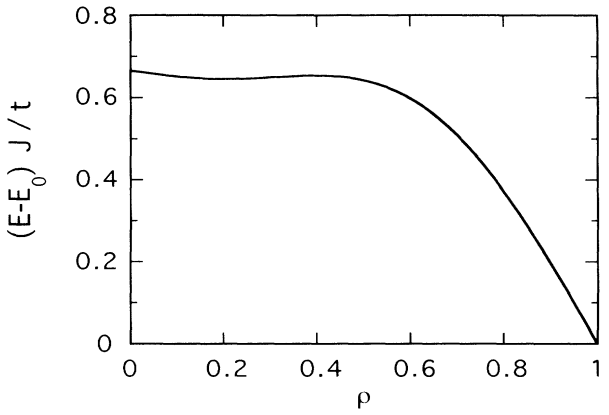

FIG. 2. Energy gain of the ferromagnetic ground state relative to the ground state of H_1 with an energy E_0 as a function of the $\tilde{f}$-electron concentration.

$$\frac{1}{\kappa}=\rho^2\left[\pi t\sin(\pi\rho)+\frac{t^2}{3J}\{(2+\rho)\pi\sin(2\pi\rho)-5[1-\cos(2\pi\rho)]\}\right], \tag{16}$$

giving the correction

$$\kappa\approx\kappa_{SF}-\frac{2t^2}{3J\rho^2}\left[(2+\rho)\cos(\pi\rho)-\frac{5}{\pi}\sin(\pi\rho)\right], \tag{17}$$

where κ_{SF} is the compressibility of noninteracting spinless Fermions. In the limit of $\rho\to 0$, the compressibility diverges as

$$\frac{1}{\kappa}\to\rho^3\pi^2 t\left[1+\frac{4t}{3J}\right], \tag{18}$$

whereas it is clear that in the insulating state at half filling κ must vanish due to the existence of a gap in the charge excitation spectrum.[19] This type of divergence of κ was noticed also for metal-insulator transitions in other systems like the Hubbard model.[20]

IV. ELEMENTARY EXCITATIONS

In this section we study among the possible elementary excitations of the system only the following two cases. The first one is the collective mode of the ferromagnetically ordered ground state, the spin-wave excitation. As a second case we consider the quasiparticle excitation of the strong-coupling KLM at half filling where the effective Hamiltonian in Eq. (3) allows a very simple treatment. The discussion of quasiparticle excitations for arbitrary filling is more complicated and will be discussed here only on a qualitative level.

A. Spin-wave excitation

The effective spin Hamiltonian [Eq. (8)] introduced in the previous section allows a very simple treatment of the spin-wave excitation on the squeezed spin chain. However, we have to clarify the relation of these excitations to the ones in the original system containing L lattice sites. Especially, we have to define the spectrum of the one-magnon spin-wave excitations in this system.

Under the assumption of periodic boundary conditions the eigenstates in the one-magnon subspace of the squeezed spin chain are given by

$$|\psi_q\rangle=\frac{1}{\sqrt{N}}\sum_{j=1}^{N}e^{iqj}S_j^-|\uparrow\cdots\uparrow\rangle \tag{19}$$

with an excitation energy

$$E_q=J_{eff}(1-\cos q)\ . \tag{20}$$

The momentum in the squeezed spin chain has the quantization $q=2\pi l/N$, l an integer with $-N/2\le l<N/2$.

In the original system the one-magnon state is written as

$$|\Psi_q\rangle=\frac{1}{\sqrt{N}}\sum_{i_1<\cdots<i_N}\sum_j\Gamma^{(0)}_{i_1,\ldots,i_N}e^{iqj}\tilde{f}^\dagger_{i_1\uparrow}\cdots\tilde{f}^\dagger_{i_j\downarrow}\cdots\tilde{f}^\dagger_{i_N\uparrow}|\mathrm{vac}\rangle\ . \tag{21}$$

The charge configuration is considered to be unaffected because we are still treating the system in the framework of first-order perturbation as done above. Thus, $\Gamma^{(0)}_{i_1,\ldots,i_N}$ is the Slater determinant in Eq. (9) for the ground state of the charge configuration in H_1. Under this condition this state [Eq. (21)] is not an eigenstate of the translation operator T which denotes the shift of complete chain by one lattice constant. A phase factor e^{iq} is occurring each time a particle is shifted through the boundary ($N\leftrightarrow 1$) and a factor 1 otherwise. Consequently, the total momentum of this state is not well defined. However, we can define the momentum in an averaged way which will

lead to the appropriate behavior in the thermodynamic limit. We operate T m times where $L/N \ll m \ll L - L/N$,

$$T^m|\Psi_q\rangle \approx e^{iqmN/L}|\Psi_q\rangle \ . \tag{22}$$

This approximate result is obtained by observing that the number of particles passing the boundary after the translation by m lattice sites is approximately $mN/L = m\rho$. In the thermodynamic limit ($L \to \infty$ and ρ fixed) this becomes exact so that the momentum $\tilde{q}$ of the spin-wave state $|\Psi_q\rangle$ is related to the momentum in the squeezed chain by $\tilde{q} = q\rho$.

In the thermodynamic limit the same relation between $\tilde{q}$ and q is obtained if the phase e^{iq} in the state in Eq. (21) is interpreted to be due to the presence of a fictitious flux threading the closed chain. This type of analysis was done in detail for the one-dimensional $U = \infty$ Hubbard model to describe the partial lift of the spin degeneracy via cyclic permutation of the spin configuration.[21] Consequently, the momenta entering in the Slater determinant are shifted accordingly, i.e., $k_j = (2\pi n_j + q)/L$ for N odd and $k_j = [\pi(2n_j+1)+q]/L$ for N even, and the matrix elements and the energy are changed slightly, since they depend on the set of momenta $\{k_1, \ldots, k_N\}$. Nevertheless, in the thermodynamic limit these changes disappear and the total momentum satisfies $\tilde{q} = q\rho$.

On the other hand, the charge excitations correspond to the creation of particle-hole pairs of $\tilde{f}$ electrons. Since in the ground state all $\tilde{f}$ electrons have the same spin, they are nothing but the particle-hole excitations of spinless fermions. These excitations are gapless at momentum 0 and $2\tilde{k}_F$. Note that $2\tilde{k}_F[=2\pi(1-n_c)]$ for the spinless fermions corresponds to $4k_{Fc}(k_{Fc} = \pi n_c/2)$, the Fermi momentum of the conduction electrons in the KLM. Within the first-order perturbation a qualitative picture of the low-energy excitations of the ferromagnetic state is summarized in Fig. 3. The one-magnon energy is zero at the same momentum, $\tilde{q} = 0$ and $2\tilde{k}_F$, as the particle-hole excitations. The energy scale of the spin-wave modes, J_{eff}, is much smaller than that of the charge

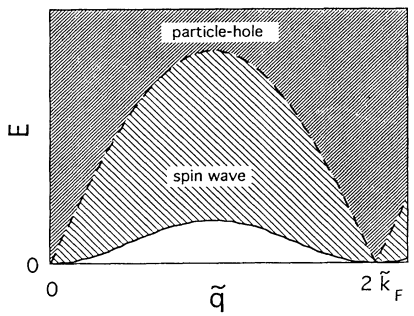

FIG. 3. Qualitative behavior of the low-energy excitation spectrum of the ferromagnetic state. The solid line marks the one-magnon spin-wave mode, whereas the dashed line stands for the lowest particle-hole excitations for a fixed momentum. The shaded areas denote the continuum of excitations, spin wave, particle hole, or both together.

excitations, t. Hence the one-magnon spin-wave branch does not enter the region of particle-hole excitations.

B. Quasiparticle excitation of the half-filled KLM

The ground state at half filling is forming an insulating state with total spin singlet, whose energy up to first order in perturbation with respect to t/J is $3J/4 + 2t^2/3J$ per lattice site.[19] In the formulation of our effective Hamiltonian [Eq. (3)], this state represents nothing but the $\tilde{f}$-electron vacuum. Hence, the quasiparticle excitation of this state is easily obtained from the one-particle eigenvalue problem

$$(E\tilde{f}_{ks}^{\dagger} - [\hat{H}, \tilde{f}_{ks}^{\dagger}])|\text{vac}\rangle = 0 \ , \tag{23}$$

where $\hat{H} = \tilde{H} - \mu N$ with N the particle number operator. We fix the chemical potential μ to zero because the half-filled system has an energy gap and zero corresponds to the center of this gap. Consequently, the quasiparticle excitation spectrum is obtained easily as

$$E_k = -t\cos k - \frac{t^2}{3J}\cos(2k) + \Delta \ , \tag{24}$$

where $\Delta = 3|J|/4 + 7t^2/12|J|$ is the charge excitation gap. This excitation is well defined in the sense that there are no modes into which it could decay. A simple quantity we can calculate immediately is the effective mass as the curvature of the quasiparticle band bottom

$$\frac{m^*}{m} = \frac{1}{1 + 4t/3J} \ , \tag{25}$$

where $m = 2t^{-1}$ denotes the mass of the spinless Fermions at $J = -\infty$, which is twice the electron mass of the original KLM. A clear enhancement of the mass can be seen with increasing value of $|t/J|$. This feature was also observed by White using results from numerical diagonalization of the KLM.[8] His and our result agree rather well for the strong-coupling regime (see Fig. 4). The deviations can be mainly attributed to finite-size effects, since White's systems are maximally 8 sites in size.

(It is easy to extend the result for the effective mass to higher dimensions by considering the number of possible paths contributing to the one-particle energy up to the order t/J in a simple hypercubic lattice. The mass enhancement is larger for higher dimensions.

$$\frac{m^*}{m} = \frac{1}{1 + 4td/3J} \ , \tag{26}$$

where d denotes the dimension.)

Finally, we note that quasiparticle and quasihole excitations show the same spectrum at half filling. Adding a conduction electron to the half-filled strong-coupling KLM leads to the break of one OSSP, since on one site two conduction electrons will form a singlet giving the localized spin free to behave as an $\tilde{f}$ electron described by the effective Hamilitonian in Eq. (3). It is easy to verify that the effective Hamiltonian has the same form above as below half filling.

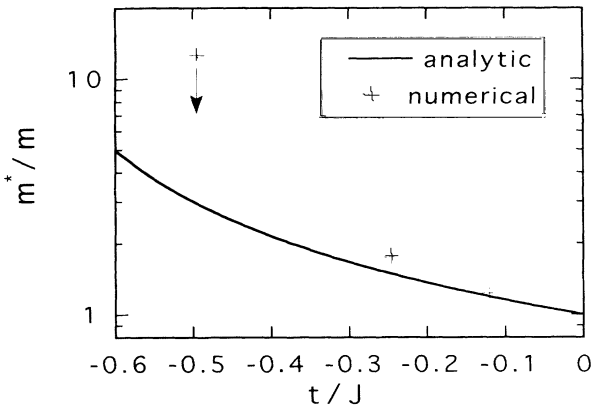

FIG. 4. Effective mass of the charge excitation at half filling. The numerical results denoted by the crosses are taken from Ref. 8. The arrow below the cross at $t/J=-0.5$ indicates that the finite-size scaling is tending towards smaller values. However, the small size of the systems does not allow a clear finite-size extrapolation in this case.

V. CONCLUSION

In this paper we introduced an effective Hamiltonian for the strong-coupling regime of the KLM, which allows one to reduce the number of degrees of freedom drastically. This Hamiltonian describes the regime in which the system consists essentially of fermions with infinitely strong on-site repulsion. We found the surprising result that the strong-coupling regime of the 1D KLM has a ferromagnetic ground state for all electron concentrations ($n_c \neq 1$).

A similar discussion of the weak-coupling regime of the KLM is considerably more difficult. The simple mapping of the KLM to a Ruderman-Kittel-Kasuya-Yosida (RKKY) system, given by

$$H_{\mathrm{RKKY}}=\sum_{j,j'}\mathcal{J}(|j-j'|)\mathbf{S}_j\cdot\mathbf{S}_{j'}\ , \tag{27}$$

in order to describe the lifting of the degeneracy of the localized spins at $J=0$ is not allowed in the 1D system. The analysis of the Fourier component of $\mathcal{J}$ shows a logarithmic singularity at $q=\pm 2k_{Fc}[k_{Fc}=\pi n_c/2;\ \tilde{\mathcal{J}}(q) \propto (J^2/q)\ln|(q-2k_{Fc})/(q+2k_{Fc})|]$. No matter how small J is chosen, the ground-state energy has no lower bound in this Hamiltonian. This indicates clearly that in weak-coupling 1D the conduction electron degrees of freedom cannot be discussed independently from that of the localized spins. Nevertheless, the $2k_{Fc}$ oscillation leading in the RKKY Hamiltonian may actually dominate the spin correlation in the weak-coupling regime for all finite conduction electron concentrations n_c. Hence, the ground state can only be ferromagnetic for vanishingly small n_c in the very weak-coupling regime. A singlet state with a strong $2k_{Fc}$ correlation in spin and charge was also observed by Troyer and Würtz in their quantum Monte Carlo calculation.[14] Similarly, Fazekas and Müller-Hartmann describe this regime by a spin spiral phase with a wave vector $Q=2k_{Fc}$.[13] In both studies no evidence was found for the formation of a large Fermi surface including conduction and localized electrons in the weak-coupling regime. However, a clear understanding of the properties of the spin singlet ground state in this regime is still missing and it is a matter of discussion whether the large Fermi surface is eventually formed at very low temperatures.

On the basis of this arguments, we conclude that the phase diagram of the 1D KLM consists of at least two phases, the ferromagnetic phase in the strong coupling limit and a spin singlet phase probably dominated by $2k_{Fc}$ correlation in charge and spin in the weak-coupling limit in the KLM. Furthermore, it was shown recently that the half-filled KLM has a spin-liquid ground state for all finite couplings J.[19]

The extension of the ferromagnetic phase into the strong-coupling region contradicts the phase diagram recently proposed by Fazekas and Müller-Hartmann, who suggest a spin singlet state in this limit exhibiting Kondo or heavy fermion state character.[13] This singlet state is described by a Gutzwiller variational wave function. Within this scheme a ferromagnetic state might appear if spin polarization as an additional degree of freedom is included into the Gutzwiller variational wave function. As far as we know this has not been examined yet.

Clearly this ferromagnetic phase in the strong-coupling regime is a special feature of the 1D system. It is well known that even on the level of the Hamiltonian H_1 [Eq. (3)] a clear difference exists between the 1D and higher-dimensional systems, for that in the latter the spin degeneracy is lifted for any band filling away from half filling ($n_c \neq 1$), e.g., favoring the Nagaoka state for $L-1$ $\tilde{f}$ electrons in an L-site lattice.[22] Concerning the extension of the ferromagnetic (Nagaoka) region in the phase diagram of higher-dimensional systems, it seems that only partially polarized ferromagnetic states might be realized for a certain range of hole concentrations.[23] Otherwise, the ground state is a total spin singlet.

On the other side, in 2D and 3D a ferromagnetic region may be more extended in the weak-coupling limit for small electron concentrations than in the 1D system. This is recognized by considering the effect of the RKKY interaction for the low-concentration limit. The oscillatory feature of this interaction is only gradually suppressing ferromagnetic order as is discussed for the 3D KLM in Ref. 11.

The effective Hamiltonian introduced in Sec. II can easily be extended to higher dimensions allowing to discuss various properties of the KLM more easily by starting from the strong-coupling regime. As a simple example we demonstrated the enhancement of the effective quasiparticle mass close to half filling. As we expect that the higher-dimensional KLM exhibits a richer phase diagram, the strong-coupling limit may provide a good starting point to approach the weak-coupling region.

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APPENDIX

For the derivation of the effective Hamiltonian it is convenient to introduce an appropriate set of operators which allow one to diagonalize the exchange part of the Hamiltonian [Eq. (1)]. We define the following operators.

$$
\begin{aligned}
b_{0i}^{\dagger} &= \frac{1}{\sqrt{2}}(f_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger} - f_{i\downarrow}^{\dagger}c_{i\uparrow}^{\dagger}) , \\
b_{1i}^{\dagger} &= f_{i\uparrow}^{\dagger}c_{i\uparrow}^{\dagger} , \\
b_{2i}^{\dagger} &= \frac{1}{\sqrt{2}}(f_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger} + f_{i\downarrow}^{\dagger}c_{i\uparrow}^{\dagger}) , \\
b_{3i}^{\dagger} &= f_{i\downarrow}^{\dagger}c_{i\downarrow}^{\dagger} , \\
d_{is}^{\dagger} &= f_{is}^{\dagger}c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger} ,
\end{aligned}
\tag{28}
$$

where $s=\uparrow$ or $\downarrow$. The operators $b_{\mu i}^{\dagger}$ create an OSSP for $\mu=0$ and an OSTP for $\mu=1$, 2, or 3, and $d_{is}^{\dagger}$ denotes the operator creating two electrons on the same site forming together a spin singlet and a localized spin s. These operators should be used with the constraint

$$
\sum_{\mu=0}^{3} b_{\mu i}^{\dagger}b_{\mu i} + \sum_{s=\uparrow,\downarrow}(f_{is}^{\dagger}f_{is} + d_{is}^{\dagger}d_{is}) = 1 \tag{29}
$$

for each site i. Note that these operators do not commute among each other in a simple way. Thus we will avoid any operation using their commutation relation.

By the use of these operators the exchange term can be written in the diagonal form

$$
H_{\mathrm{ex}} = \frac{3}{4}J\sum_{i} b_{0i}^{\dagger}b_{0i} - \frac{1}{4}J\sum_{i}\sum_{\mu=1}^{3} b_{\mu i}^{\dagger}b_{\mu i} . \tag{30}
$$

Obviously, the exchange term is zero in the case of an empty or doubly occupied site. For this simplicity in the exchange term we have to pay with a more complicated structure of the hopping term.

$$
\begin{aligned}
H_{\mathrm{kin}} &= -t\sum_{i,j,s} c_{is}^{\dagger}c_{js} + \mathrm{H.c.} \\
&= -t\sum_{i,j,s}\left\{\left[\sum_{s_1} f_{is_1}^{\dagger}f_{is_1}\right]\left[\sum_{s_2}(c_{is_2}^{\dagger}c_{is_2} + c_{is_2}c_{is_2}^{\dagger})\right]c_{is}^{\dagger}c_{js}\left[\sum_{s_3}(c_{js_3}^{\dagger}c_{js_3} + c_{js_3}c_{js_3}^{\dagger})\right]\left[\sum_{s_4} f_{js_4}^{\dagger}f_{js_4}\right] + \mathrm{H.c.}\right\} ,
\end{aligned}
\tag{31}
$$

where we multiplied several unities to the original Hamiltonian. Proceeding by appropriate commutation of f and c operators $\mathcal{H}_{\mathrm{kin}}$ reaches the form

$$
\begin{aligned}
H_{\mathrm{kin}} = -t\sum_{i,j}\sum_{s_1,s_2,s_3}\Bigg[& \left[\sum_{s'} c_{is'}c_{is'}^{\dagger}\right](f_{is_2}^{\dagger}c_{is_1}^{\dagger})f_{is_2}f_{js_3}^{\dagger}(c_{js_1}f_{js_3})\left[\sum_{s''} c_{is''}c_{is''}^{\dagger}\right] \\
& + \mathrm{sgn}(s_1)(f_{js_2}^{\dagger}c_{is_1}^{\dagger}c_{i,-s_1}^{\dagger})(c_{is_1}f_{is_2})f_{js_3}^{\dagger}(c_{j,-s_1}f_{js_3})\left[\sum_{s'} c_{is'}c_{is'}^{\dagger}\right] \\
& + \mathrm{sgn}(s_1)\left[\sum_{s'} c_{is'}c_{is'}^{\dagger}\right](f_{is_2}^{\dagger}c_{i,-s_1}^{\dagger})f_{is_2}(f_{js_3}^{\dagger}c_{js_1}^{\dagger})(c_{j,-s_1}c_{js_1}f_{js_3}) \\
& + (f_{js_2}^{\dagger}c_{is_1}^{\dagger}c_{i,-s_1}^{\dagger})(c_{is_1}f_{is_2})(f_{js_3}^{\dagger}c_{js_1}^{\dagger})(c_{j,-s_1}c_{js_1}f_{js_3}) + \mathrm{H.c.}\Bigg] ,
\end{aligned}
\tag{32}
$$

where $\mathrm{sgn}(s)=+1$ for $s=\uparrow$ and $=-1$ for $s=\downarrow$. In this expression we can replace the combination in the brackets by the new operators keeping the imposed constraint in Eq. (29).

$$
\begin{aligned}
H_{\mathrm{kin}} = -t\sum_{i,j}\Bigg\{ & \frac{1}{2}\sum_{s}[b_{2i}^{\dagger} - \mathrm{sgn}(s)b_{0i}^{\dagger}]\tilde{f}_{is}\tilde{f}_{js}^{\dagger}[b_{2j} + \mathrm{sgn}(s)b_{0j}] + b_{1i}^{\dagger}\tilde{f}_{i\uparrow}\tilde{f}_{j\uparrow}^{\dagger}b_{1j} + b_{3i}^{\dagger}f_{i\downarrow}f_{j\downarrow}^{\dagger}b_{3j} \\
& + 2\Bigg[\frac{1}{\sqrt{2}}b_{1i}^{\dagger}\tilde{f}_{i\uparrow}\tilde{f}_{j\downarrow}^{\dagger}(b_{2j} - b_{0j}) + \frac{1}{\sqrt{2}}(b_{0i}^{\dagger} + b_{2i}^{\dagger})\tilde{f}_{i\uparrow}\tilde{f}_{j\downarrow}^{\dagger}b_{3j} \\
& - \left[d_{i\uparrow}^{\dagger}b_{1i} + \frac{1}{\sqrt{2}}d_{i\downarrow}^{\dagger}(b_{2i} - b_{0i})\right]\left[\tilde{f}_{j\downarrow}^{\dagger}b_{3j} + \frac{1}{\sqrt{2}}\tilde{f}_{j\uparrow}^{\dagger}(b_{0j} + b_{2j})\right] \\
& + \left[\frac{1}{\sqrt{2}}d_{i\uparrow}^{\dagger}(b_{0i} + b_{2i}) + d_{i\downarrow}^{\dagger}b_{3i}\right]\left[\tilde{f}_{j\uparrow}^{\dagger}b_{1j} + \frac{1}{\sqrt{2}}\tilde{f}_{j\downarrow}^{\dagger}(b_{2j} - b_{0j})\right] \\
& + \left[d_{i\uparrow}^{\dagger}b_{1i} + \frac{1}{\sqrt{2}}d_{i\downarrow}^{\dagger}(b_{2i} - b_{0i})\right]\left[b_{1j}^{\dagger}d_{j\uparrow} + \frac{1}{\sqrt{2}}(b_{2j}^{\dagger} - b_{0j}^{\dagger})d_{j\downarrow}\right] \\
& + \left[\frac{1}{\sqrt{2}}d_{i\uparrow}^{\dagger}(b_{0i} + b_{2i}) + d_{i\downarrow}^{\dagger}b_{3i}\right]\left[b_{3j}^{\dagger}d_{j\downarrow} + \frac{1}{\sqrt{2}}(b_{0j}^{\dagger} + b_{2j})d_{j\uparrow}\right]\Bigg] + \mathrm{H.c.}\Bigg\} ,
\end{aligned}
\tag{33}
$$

where we introduced $\tilde{f}$ operators for the sites with a localized spin but no conduction electron, $\tilde{f}_{is}^{\dagger}=(1-n_{ci})f_{is}^{\dagger}$ with $n_{ci}=\sum_s c_{is}^{\dagger}c_{is}$. Although the structure of these hopping terms is much more complicated than that of the original one, this form is often more convenient for various types of calculations, for example, cluster expansions.

We derive now an effective Hamiltonian for the strong-coupling limit by a canonical transformation

$$\tilde{H}=e^{-S}He^{S} \tag{34}$$

to eliminate all terms containing operators other than $b_{0i}^{(\dagger)}$ and $\tilde{f}_{is}^{(\dagger)}$. This is equivalent to a perturbation with $H_{\rm kin}$ as the perturbative Hamiltonian to lift the degeneracy of the lowest-energy eigenstates of $H_{\rm ex}$ in charge and spin configuration space. The result of this straightforward procedure is

$$\begin{aligned}\tilde{H}=&-\frac{t}{2}\sum_{i,s} b_{0i}^{\dagger}\tilde{f}_{is}\tilde{f}_{i+1,s}^{\dagger}b_{0,i+1}+\frac{t^2}{2J}\sum_{i,s,s'} b_{0,i-1}^{\dagger}\tilde{f}_{i-1,s}\tilde{f}_{i,s'}^{\dagger}\tilde{f}_{i,s'}\tilde{f}_{i+1,s'}^{\dagger}b_{0,i+1}-\frac{t^2}{4J}\sum_{i,s,s'} b_{0,i-1}^{\dagger}\tilde{f}_{i-1,s}\tilde{f}_{is'}^{\dagger}\tilde{f}_{is'}\tilde{f}_{i+1,s}^{\dagger}b_{0,i+1}\\&+\frac{t^2}{6J}\sum_{i,s} b_{0,i-1}^{\dagger}\tilde{f}_{i-1,s}b_{0i}^{\dagger}b_{0i}\tilde{f}_{i+1,s}^{\dagger}b_{0,i+1}+\frac{3t^2}{4J}\sum_{i} b_{0i}^{\dagger}b_{0i}-\frac{5t^2}{12J}\sum_{i} b_{0i}^{\dagger}b_{0i}b_{0,i+1}^{\dagger}b_{0,i+1}+\frac{3J}{4}\sum_{i} b_{0i}^{\dagger}b_{0i}+\text{H.c.}\,,\end{aligned} \tag{35}$$

where we keep the constraint $\sum_s \tilde{f}_{is}^{\dagger}\tilde{f}_{is}+b_{0i}^{\dagger}b_{0i}=1$ for all sites i. Since the operators b_0 can be understood as a hole in a system of $\tilde{f}$ electrons only, they can be dropped in this Hamiltonian, keeping the $\tilde{f}$ operators only with the constraint that no double occupancy is allowed for the $\tilde{f}$ electrons. This leads to the effective Hamiltonian given in Eq. (3).

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