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Falicov-Kimball model and its relation to the Hubbard model: Studies on clusters

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Ground-state properties of the asymmetric Hubbard model are studied on one-dimensional clusters (rings) with $N = 6$, 8, and 10 sites. The ground-state energy, correlation functions, and phase diagrams are determined for various sets of model parameters. Computations are performed both by exact diagonalization (for $N = 6$) and by an approximate method by which correlation effects can be examined on larger clusters than exact diagonalization allows. In the limiting cases (one limit corresponds to the spinless Falicov-Kimball model and the other to the Hubbard model) our results agree quite well with those obtained analytically for infinite systems.

I. INTRODUCTION

The Falicov-Kimball model (FKM) in its spinless version can be regarded as a modification of the one-band Hubbard model[1,2] (HM) in which the electrons with one spin direction possess infinite masses and hence do not move while those with the other spin direction are free to move. For this reason the model is also called the static HM.[2] This seems to be the simplest, nontrivial model of correlated electron systems (there are also other physical interpretations[3,4]) where many-body effects are clearly manifested. The FKM is defined on a lattice of N sites by the Hamiltonian

$$H_{\rm FKM} = -\sum_{\langle k,l\rangle} d_k^\dagger d_l + U\sum_k d_k^\dagger d_k f_k^\dagger f_k, \qquad (1)$$

where the hopping term of the moving electrons is summed over all nearest-neighbor (NN) lattice sites $\langle k,l\rangle$; $d_k(d_k^\dagger)$ and $f_k(f_k^\dagger)$ are, respectively, the annihilation (creation) operators for the itinerant and localized electrons at site k (hereafter, the former are called electrons and the latter, ions); U is the electron-ion on-site Coulomb interaction. The electron hopping integral is taken to be the unit of energy. Here we consider the case of a repulsive electron-ion interaction $U \geq 0$; the case $U < 0$ can be treated by using the symmetry of the Hamiltonian (1).[4] There are $N_e = \sum_k d_k^\dagger d_k$ electrons and $N_i = \sum_k f_k^\dagger f_k$ ions in the system. The corresponding densities are $\rho_e = N_e/N$ and $\rho_i = N_i/N$; $N_e + N_i \leq 2N$.

During the last few years, a number of exact[2,5] or well-controlled approximate results have been obtained for this model. Most of these concern ground-state properties on one-dimensional[4,6-10] ($d = 1$) or two-dimensional lattices.[3,5,11,12] In particular they show that in the ground state the ions are ordered in a definite pattern which depends on values of the model parameters. The zero-temperature phase diagram within the canonical ensemble[4] (the case of the grand canonical ensemble was investigated in Refs. 6 and 13) appears to be separated generally into three distinct regions: (i) the most homogeneous ionic configurations (in the sense of Ref. 8) — for U large enough and $\rho_e = 1 - \rho_i$, (ii) the so-called segregated configuration where the ions clump together — for U large enough and $\rho_e \neq 1 - \rho_i$, (iii) the complex (fractal-like) structure where the configuration of the ions changes point by point at every value of the electron concentration and $\rho_e \neq 1 - \rho_i$.

In this contribution we extend our studies to the generalized spinless FKM (asymmetric HM)[14] in which both the electrons and the ions are allowed to jump between the nn sites. Thus we deal with the Hamiltonian

$$H = H_{\rm FKM} - t\sum_{\langle k,l\rangle} f_k^\dagger f_l, \qquad (2)$$

where t is the ionic hopping integral between the nn sites $\langle k,l\rangle$. The model under consideration corresponds to the situation where Coulomb energies for two particles of the same sort are too great to allow them to occupy the same site, whereas the energy remains finite and equal to U for an electron and an ion on the same site. This model can be viewed not only as a generalized spinless FKM but also as a generalized one-band HM. Both these models can be obtained from Eq. (2) with a special choice of the model parameters, namely: $t = 0$ gives the spinless FKM and $t = 1$ gives the HM. The results we report here were obtained on $d = 1$ clusters (rings) with $N = 6, 8$, and 10 sites. Even such small finite systems have properties which reflect quite well those of corresponding infinite systems in limiting cases where they are known exactly (see Sec. III). The purpose of our studies is twofold: (i) to find out how the ground-state characteristics of the system change when the localized electrons start to move, (ii) to introduce and test a method by which one can study many-body effects at $T = 0$ for systems larger than those attainable by exact diagonalization. The idea of describing the HM starting from the FKM has already been explored but only for $d = \infty$ (mean field) and rather large U.[15] In our approach a small U is an advantage. Since the method is not perturbative, it does not give a quantitative estimate of the limits within which it is valid. We would point out however that the approximation used is exact not only for $t = 0$ but also for $U = 0$

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when the two subsystems (electronic and ionic) are decoupled. Thus the method would be expected to give reasonable results for small U, as numerical calculations in fact confirm. We plan to study this point in a later paper. The ground-state properties of the system are described in terms of correlation functions and probabilities of particular ionic configurations. In the next section, we define the quantities that we calculate and describe our method; the results are presented in Sec. III; Sec. IV contains our conclusions.

II. METHOD OF CALCULATION

The Hamiltonian (2) is considered in a basis of localized states, i.e., states which are eigenstates of the occupation number operators of the electrons $n_k^e = d_k^\dagger d_k$ and the ions $n_k^i = f_k^\dagger f_k$. We note that the total numbers of the electrons N_e and the ions N_i are good quantum numbers, so the Hamiltonian (2) can be diagonalized in subspaces with fixed values of N_e and N_i. For a given N-site cluster containing N_e electrons and N_i ions there are $\binom{N}{N_e}$ electronic and $\binom{N}{N_i}$ ionic states, hence the dimension of the matrix for diagonalization is equal to $\binom{N}{N_e} \cdot \binom{N}{N_i}$.

We define the electron-electron (L_{ee}), the ion-ion (L_{ii}) and the electron-ion (L_{ie}) correlation functions by

$$L_{ab}(x) = \frac{1}{N}\left\langle 0 \left| \sum_{|k-l|=x} n_k^a n_l^b \right| 0 \right\rangle, \qquad (3)$$

where $|\,0\rangle$ is the ground state of the system and x denotes the distance between the sites. Suffixes a, b indicate the electron and the ion, respectively.

Any ionic phase of the system represents a class of those configurations of the ions which are related by cluster symmetries. As a result, the probability $P\{n_i\}$ of a given ionic phase is calculated by summing the probabilities of all those states of the system which belong to a relevant class. The number of states represented by a given phase depends on many factors such as the size and geometry of the cluster, the numbers of ions and electrons present in the system as well as the type of arrangement of the ions. For example for $d = 1$ with periodic boundary conditions there are $N \cdot \binom{N}{N_e}$ states corresponding to the segregated phase, i.e., there are $\binom{N}{N_e}$ electronic states for each of the N ionic configurations related by translation. We have calculated $L_{ab}(x)$, $P\{n_i\}$ and the ground-state energy E_0 (see Sec. III).

Usually calculations on clusters are performed by exact diagonalization.[16] The task becomes very difficult because the number of states increases very rapidly with the number of sites involved. To overcome this we propose an approximate method relevant at zero and possibly also at very low temperatures. Our method consists of two steps. (1) We find the lowest-energy state for every permissible ionic configuration (as in the pure spinless FKM case). To do this we must diagonalize matrices of rank $\binom{N}{N_e}$, which correspond to particular ionic configurations. (2) We take the states thus found as a basis of a new matrix [of rank $\binom{N}{N_i}$] which we subsequently diagonalize. At the first stage we divide the full Hilbert space into $\binom{N}{N_i}$ subspaces [each of dimension $\binom{N}{N_e}$] and we find the exact ground state within each of the subspaces. These many-body ground states form a new basis for a matrix whose rank is only $\binom{N}{N_i}$ and which approximately describes the properties of the initial system.

A physical justification of the method arises naturally from the fact that we deal with two different sorts of fermionic particles: slow ones (ions) and fast ones (electrons). A crucial point consists in the assumption that between every ion jump the system attains its lowest energy state adequate for a given temporary configuration of the ions. In fact, our procedure is similar to the Born-Oppenheimer or adiabatic approximation used in molecular physics and chemistry.[17]

Such an approximation — which is exact for $t = 0$ — is expected to be reasonable if the kinetic energy of the ions is small compared to that of the electrons, i.e., for $t \ll 1$. Surprisingly however, it works quite well even for $t = 1$ (HM case) if $U < 1$. Indeed, all the ground-state characteristics of the systems calculated by an exact diagonalization are reproduced by the approximate method not only qualitatively but also — within a small relative error — quantitatively for the whole range of values of t, i.e., for $0 \leq t \leq 1$, if $U < 1$.

III. RESULTS

A. Phase diagrams

Since we are interested in the stability of the ionic ordering with respect to the kinetic energy term of the ions, we have calculated the probabilities of particular ionic configurations. The probability of an ionic phase at the temperature $T = 0$ is calculated by a projection of the ground-state wave function onto the subspace of ionic states within a given equivalence class. We performed the calculations for a large set of model parameters $U, t, N_i, N_e, (N \leq 10)$ and we constructed phase diagrams in the variables (U, t). The phases presented in the phase diagrams are those with the highest probabilities for given values of U and t. Examples of such diagrams for $N = 8$ and for some typical values of $N_i (= N_e)$ are displayed in Figs. 1 and 2.

A general feature which can be noticed in these pictures is that the arrangement of the ions is stable with respect to their kinetic energy, but only for a rather small interval of values of t.

A second observation is that in each diagram the largest part belongs to that phase that is the most probable one for $t = 1$ (HM). One can conclude that the ions show evidence of ordering where t is small enough and U large. In the case of $N_i = N_e = 4$ an effective repulsion between the ions persists for all values of U, provided t is sufficiently small. On the other hand, for $N_i = N_e < 4$, the region in which the most probable distribution of the ions differs from that found in the limit $t = 1$ (HM), may begin at a certain $U = U_c > 0$.

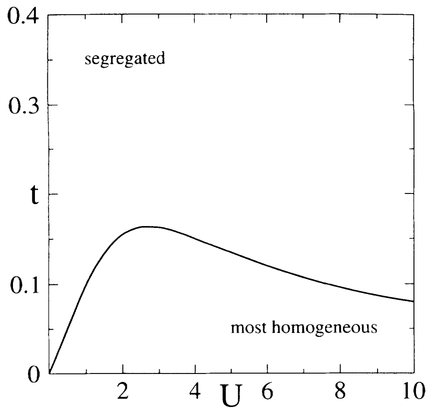

FIG. 1. The $T = 0$ phase diagram as a function of U and t for $N = 8$, $N_i = N_e = 4$. U: electron-ion on-site Coulomb interaction; t: ionic hopping integral between NN sites. U and t are in units of the electron hopping integral. "Most homogeneous" and "segregated" phases refer to the ionic configurations described in Sec. I. The most homogeneous configuration is [○ ● ○ ● ○ ● ○●] and the segregated configuration is [● ● ● ● ○ ○ ○○]. (Empty sites are represented by ○, occupied sites by ●.)

Our calculations also indicate the possibility of the appearance of a few intermediate phases (see Fig. 2) related to a gradual rearrangement of the ions when t increases from $t = 0$ and $U > U_c$.

Let us now regard these diagrams from the point of view of an effective interaction between the ions. Among various possible phases, i.e., ionic configurations, there are two special ones: the segregated and the most homogeneous classes. The former corresponds to an effective attraction and the latter to an effective repulsion between the ions. Thus, for a certain set of model parameters ($U > U_c, t \ll 1, N_i = N_e \neq N/2$) an effective attraction between the ions exist. It is interesting that in a pure electronic system (without phonons) and with only a single-site Coulomb repulsion between ions and electrons in the initial Hamiltonian, an effective attraction between the ions is produced. This property arises strictly from correlation effects present in the system.

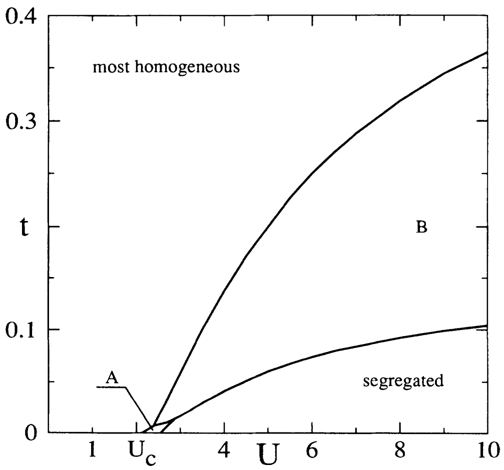

FIG. 2. The $T = 0$ phase diagram as a function of U and t for $N = 8$, $N_i = N_e = 3$. Notation as in Fig. 1. The phase A is [● ● ○ ● ○ ○ ○○], the phase B is [● ● ○ ○ ● ○ ○○], and the most homogeneous phase is [● ○ ○ ● ○ ○ ●○]. $U_c = 2.212\,28$.

B. The double occupancy

The on-site electron-ion correlation $L_{\rm ie} \equiv L_{\rm ie}(x = 0)$ which is equal to the probability that a given site is occupied by both an ion and an electron (a double occupancy) is another parameter that characterizes the state of correlated electrons. In the HM limit this quantity is related to the magnitude of the local magnetic moments[20] $S_0 = (1/N)\langle 0 \mid \sum_k (S_k)^2 \mid 0\rangle$, where S_k is the spin operator at the kth site and the average is taken in the ground state. On the other hand, L_{ie} is also related to the Gutzwiller variational parameter[18] g which governs the number of double occupied sites.

The behavior of $L_{\rm ie}$ as a function of t for a few values of U and $N_i = N_e (N = 8)$ is displayed in Fig. 3. Two conclusions arise from Fig. 3: (i) $L_{\rm ie}$ decreases when U increases or when the number $N_i (= N_e)$ decreases. (ii) $L_{\rm ie}$ is almost independent of t for t larger than a certain, rather small t^* which depends on U. Quite unexpectedly,

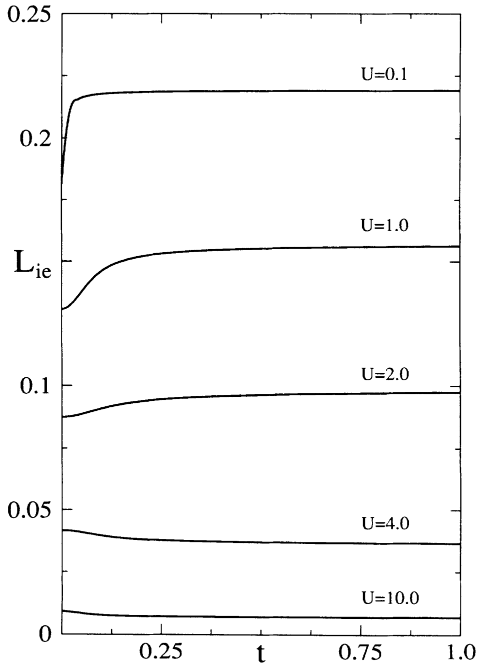

FIG. 3. Ground-state electron-ion correlation function $L_{\rm ie}$ [Eq. (3)] calculated by the approximate method developed in the text for the system with $N = 8$ and $N_i = N_e = 4$. U: electron-ion on-site Coulomb interaction; t: ionic hopping integral between NN sites. U and t are in units of the electron hopping integral.

L_{ie} remains dependent on t near $t = 0$. For $N_i = N_e = 4$ and a small U, L_{ie} increases with t, but for a large enough U it decreases with t (see Fig. 3). At present we are not able to explain this strange behavior, possibly it is related to the rearrangement of the ions in proximity to the spinless FKM limit.

C. The correlation functions

For $N = 6$ we have calculated exactly the electron-electron L_{ee} and the ion-ion L_{ii} correlation functions between first, second, and third neighbors, and we show them in Fig. 4. Insets in Fig. 4 represent these functions calculated by the approximate method.

A striking property is a negligible dependence of the L_{ee} function on t whereas L_{ii} changes significantly with t. This means that slower ions have almost no influence on the movement of the electrons. The correlations L_{ee} are modified only, and even then only slightly, if U is large enough and t is small. This is in opposition to the case of the slow ions ($t \ll 1$) whose motion is strongly perturbed by the presence of fast electrons. In the limit $t = 1$ (HM) and for $N_i = N_e$ the ion-ion and the electron-electron correlation functions are equal to each other, i.e., $L_{ii}(x) = L_{ee}(x)$ as it should be by the symmetry between electrons and ions. This property is reproduced by the approximate method we used.

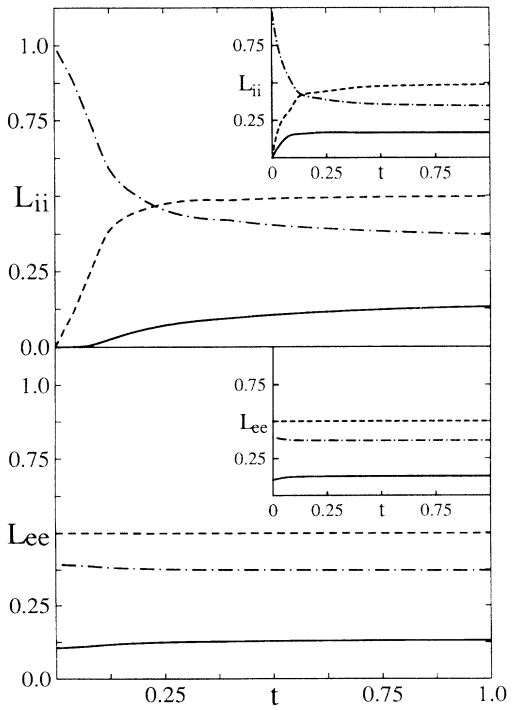

FIG. 4. First-neighbor (solid line), second-neighbor (dashed line), and third-neighbor (dash-dotted line) electron-electron (L_{ee}) and ion-ion (L_{ii}) ground-state correlation functions [see Eq. (3)] calculated exactly for $N = 6$, $N_i = N_e = 2$ and $U = 1$. Notation as in Fig. 3. Insets show these functions calculated by the approximate method.

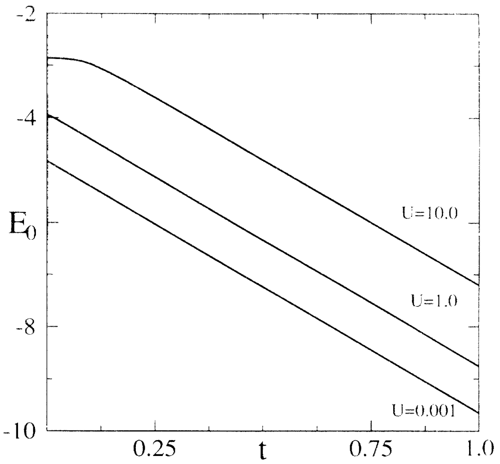

FIG. 5. Ground-state energy E_0 as a function of t calculated by the approximate method. $N = 8$, $N_i = N_e = 3$. Notation as in Fig. 3.

D. Ground-state energy

To check our results we calculated the total energy per site of the system. The ground-state energy as a function of t for three representative values of U (0.001, 1.0, 10.0) is shown in Fig. 5. A characteristic feature of this function is its linearity for a great part of the interval of t values. Departure from the linearity is observed only for small t and large U. This is probably connected with the regrouping of the ions which tend to set up their appropriate positions to achieve the ground-state configuration.

In the limiting cases of $t = 1$ and $t = 0$ we compare our exact and approximate ground-state energies for finite systems with those obtained for infinite[19] HM and spinless[2] FKM, respectively (see Table I and Table II). The method we use is not variational thus it is not surprising that the energy calculated approximately is lower than the exact value. Actually, the lower bound for the ground-state energies of the HM have already been obtained by other methods.[22]

We noticed that the energy per site calculated by the approximative method for $t = 1$ is close to the energy obtained both from exact diagonalization studies on finite systems[20] and from the exact $d = 1$ infinite system[21]

TABLE I. Ground state energy (per site) of the HM ($t = 1$). $N_i = N_e = N/2$.

	Exact	Approximate method		Analytical[a]
U	$N = 6$	$N = 6$	$N = 10$	$N = \infty$
0.1	-1.30850	-1.30868	-1.26978	-1.27074
1.0	-1.10019	-1.11770	-1.08013	-1.04037
10.0	-0.27739	-0.73823	-0.71753	-0.26716

[a] Reference 19.

TABLE II. Ground state energy (per site) of the FKM ($t = 0$). $N_i = N_e = N/2$.

	Exact and approximate method		Analytical[a]
U	$N = 6$	$N = 10$	$N = \infty$
0.1	-0.64219	-0.62283	-0.61273
1.0	-0.46627	-0.45385	-0.45142
10.0	-0.09720	-0.09718	-0.09718

[a] Reference 7.

for $U < 1$. However, the differences between energies calculated by the exact and by the approximate methods increase with U. From this observation we conclude that our approximate approach seems to work well for small values of U, at least when the HM limit is investigated (if t is smaller, then the approximation works well even for larger U).

IV. CONCLUSIONS

We have studied the asymmetric Hubbard model on one-dimensional clusters (rings) by an exact diagonalization and an approximate method. The method we used (see Sec. II) takes into account essential features of the correlated electron state and enables us to study larger clusters than the exact diagonalization method does. In particular, ground-state energies, correlation functions, and probabilities of ionic configurations obtained by the exact diagonalization method are very close to each other for small values of t or U. What is more, the ground-state energies per site for finite systems are found to be very close to those for the $d = 1$ infinite spinless FKM ($t = 0$) and, surprisingly, even to those for the $d = 1$ HM ($t = 1$), although only if $U < 1$. Thus we think that the ground-state properties of clusters are in many respects typical of infinite systems, and that our studies give reliable insight into the nature of certain correlated electron systems. Our findings may be summarized as follows. (i) Properties of the spinless FKM change smoothly when the ions start to move. (ii) Correlation functions between the electrons are almost independent of the kinetic energy of the ions; they only change a little in the region of large U and small t values. (iii) Correlation functions between the ions are strongly dependent on t for all values of U, especially for small values of t.

Consequently, we can say that the motion of the slow particles is strongly influenced by the fast ones, but the converse statement is not true: the fast particles are almost unaffected by the presence of the slow ones.

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