Ground states of the Falicov-Kimball model with correlated hopping

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Two-dimensional spinless Falicov-Kimball model (FKM) with correlated hopping is studied perturbatively in the limit of large on-site Coulomb interaction U. In the half filled case (i.e., $\rho_i + \rho_e = 1$, where ρ_i, ρ_e are densities of ions and electrons, respectively) the effective Hamiltonian in spin variables is derived up to terms proportional to U^{-3}. Unlike the simplest FKM case, it contains odd parity terms (resulting from the correlated hopping) in addition to even parity ones. The ground-state phase diagram of the effective Hamiltonian is examined in the $(a/t, h)$ plane, where a/t is a parameter characterizing strength of the correlated hopping and h is a difference of chemical potentials of two sorts of particles present in the system. It appears to be asymmetric with respect to the change $h \rightarrow -h$ and an additional ordered phase is found for a certain interval of a/t.

I. INTRODUCTION

One of the most fascinating, but still mysterious phenomenon observed in some materials is a charge ordering.[1] Despite of its oddity, originated from the quantum nature of interacting electrons, it seems to be very likely that an inhomogeneous charge distribution is a very common effect present in strongly correlated electron systems.[2] Then, presumably, it must be related to a number of various phenomena found in the systems (such as *metal-insulator phase transition, high-T_c superconducitivity, giant magnetoresistivity*, just to mention a few). The above arguments point out how important is the understanding of the nature of the effect and justify growing interest in its theoretical description.[2] In particular it is important to determine factors deciding about what sorts of charge superstructures are formed.

One of the simplest models suitable to decribe charge-ordered phases on a microscopic level is the Falicov-Kimball model (FKM), previously applied to account for the metal-insulator transition,[3] mixed valence phenomena,[4] crystallization and alloy formation,[5] etc. Indeed, it was shown that ground-state phase diagrams of the simplest version of the FKM have extremely rich structure.[6-8] The great advantage of the model is that it is amenable to rigorous analysis.[9,10]

However, the simplest version of the FKM, although nontrivial, is not able to account for all aspects of real experiments. An objective of our studies is the gradual inclusion of those terms that were ignored in the simplest version of the FKM, yet keeping the model tractable.

In this contribution we investigate the FKM with the so-called *correlated hopping term* added (chFKM). This term was already mentioned by Hubbard in Ref. 11. More than a decade ago Hirsch pointed out that the term may be relevant in the explanation of superconducting properties of strongly correlated electron systems (he named it *the bond-charge interaction*).[12] In the past few years some other authors have examined a role of the correlated hopping in the FKM,[13] and the Hubbard model,[14,15] mainly in the context of the metal-insulator phase transition. Inclusion of this term makes electron hopping rate dependent on occupation numbers of those

sites between which an electron hops.

One of the most difficult problems that one encounters, when trying to describe correlated electron systems, is the choice of a reliable method that enables us to treat the model under consideration in a controllable way. Here we use a perturbative method valid in the large U limit, that permits us to transform an initial Hamiltonian, having a small quantum part, into an effective classical one. The method has been reported in a series of papers by Datta, Fernandez, Fröhlich, and Rey-Bellet.[16-19] One can use this method to generate a perturbative series up to an arbitrarily high order in $1/U$, to establish the *convergence* of the whole procedure, and—in some cases—to obtain phase diagrams in low (but nonzero) temperatures. This can be done by extending the techniques of Pirogov-Sinai theory[20] to quantum models.

The aim of our paper is to examine properties of the chFKM in the *perturbative regime*, i.e., in the range of parameters where all kinds of hopping terms are small in comparison with the on-site Coulomb interaction term U. We are particularly interested in the examination of how the correlated hopping term influences charge ordering. In the first part of our work we derived an effective Hamiltonian, that is legitimated in the large U limit. Then we found its ground-state properties by means of the method of restricted phase diagrams, used previously in the simplest version of the FKM.[7,8]

II. MODEL

We are dealing with two types of particles defined on a d-dimensional simple cubic lattice $\mathbf{Z}^d$: immobile ions and itinerant spinless electrons. (other interpretations of the model have also been considered[5,7-9]).

The Hamiltonian defined on a finite subset Λ of $\mathbf{Z}^d$ has the form

$$H_\Lambda = H_{0,\Lambda} + V_\Lambda, \tag{1}$$

where

64 233103-1

$$H_{0,\Lambda} = U \sum_{x \in \Lambda} w_x n_x - \mu_i \sum_{x \in \Lambda} w_x - \mu_e \sum_{x \in \Lambda} n_x, \qquad (2)$$

$$V_\Lambda = -\sum_{\langle xy \rangle} [t + a(w_x + w_y)](c_x^\dagger c_y + c_y^\dagger c_x). \qquad (3)$$

Here $c_x^\dagger$ and c_x are creation and annihilation operators of an electron at lattice site $x \in \Lambda$, satisfying ordinary anticommutation relations and the corresponding number particle operator is $n_x = c_x^\dagger c_x$. w_x is a classical variable taking values 0 or 1. It measures the number of ions at lattice site x. The chemical potentials of the ions and electrons are μ_i and μ_e, respectively, t is the electron hopping amplitude between empty sites and a is the correlated hopping constant. The symbol $\langle xy \rangle$ denotes an orderless pair of nearest-neighbor sites of the lattice.

In this paper we examine the model in the range of parameters $t, a \ll U$. The value of a is usually smaller than that of t, however, both these quantities are of the same order. Indeed, in systems described by the Hubbard-like models, it has been found that $|a/t| \approx 0.3$.[11,12] In our studies we impose the following condition: $-t \leqslant a \leqslant t$ (for $a = 0$, this model reduces to the ordinary FKM).

III. GENERAL OUTLINE OF THE PERTURBATION SCHEME

The perturbative scheme we use here can be applied to a general class of (lattice) Hamiltonians (defined on $\Lambda \subset \mathbf{Z}^d$) of the following form:

$$H_\Lambda(t) = H_{0,\Lambda} + rV_\Lambda, \qquad (4)$$

where the unperturbed Hamiltonian $H_{0,\Lambda}$ is a *classical* operator (i.e., it is diagonal in a basis being the product of bases on all lattice sites) with degenerate ground states. (Obviously the chFKM, introduced by the formulas above, belong to this class.) Our purpose is to examine the effect of a quantum perturbation rV_Λ, where r is a small parameter. In other words, we want to (block) diagonalize the Hamiltonian and find its ground states.

To accomplish this task we are looking for a unitary transformation $U(r)$, which (block) diagonalizes the full Hamiltonian. In most cases, finding out such a transformation exactly is a hopeless job. More constructive method is a *perturbative* treatment, consisted in "killing" the off-diagonal part of perturbation up to some finite power of the parameter r:

$$H(r) \equiv H_0 + rV \rightarrow \tilde{H}_0^{(n)}(r) + r^{n+1}\tilde{V}^{od},$$

where $\tilde{H}_0^{(n)}(r)$ is block diagonal up to the order $n+1$ in r. In this way one can determine an explicit formula for a diagonal part of the perturbed Hamiltonian $\tilde{H}_0^{(n)}(r)$, called the effective Hamiltonian.

Results based on various perturbative schemes have been previously obtained for the simplest versions (i.e., without correlated hopping term) of the FKM and Hubbard models.[19,21,22] The method applied in our studies was devel-

oped in Refs. 16–19 for Hamiltonians of the form (4). Their components can have a quite general form; it is sufficient that both of them are sums of finite range operators (or even infinite-range but exponentially decreasing with distance). Moreover, it is assumed that H_0 is expressible by translationally invariant m potential.[17,18,23]

The technique developed in Refs. 16–19 has also two other important aspects. First, since we restrict ourselves to the low-temperature region of the phase diagram, we need to diagonalize only *a low-energy* part of the Hamiltonian, which considerably simplifies the calculations. Second, special care is taken to the form of the transformed Hamiltonian: it is formulated as a sum of *local* operators. It is necessary to obtain uniform estimates (i.e., independent of volume) and, as a consequence, to establish the convergence of the whole procedure, and (in some cases) to examine orderings emerging in the system.

All this formalism, its background, achievements, and limitations can be found in Refs. 16–19. It must be stressed that many analogous results have been also obtained by Kotecky and co-workers.[24,25]

IV. EFFECTIVE HAMILTONIAN

The Hilbert space of the whole system $\mathcal{H}_\Lambda$ is a tensor product: $\mathcal{H}_\Lambda = \otimes_{x \in \Lambda} \mathcal{H}_x$. Every $\mathcal{H}_x$ is spanned by the states: $|w_x, n_x\rangle$. There are four base vectors: $|0,0\rangle$, $|1,0\rangle$, $|0,1\rangle$, and $|1,1\rangle$. The corresponding energies are: $0; -\mu_i; -\mu_e; U - \mu_i - \mu_e$.

Let us begin our analysis from the classical part of the Hamiltonian. It is identical to a classical part of the Hubbard model and the FKM, and it is well known.[19] The phase diagram consist of four regions. In region *I*, defined by $\mu_i < 0, \mu_e < 0$, all sites are empty. In two twin regions II_i, II_e, given by the conditions II_i: $\mu_i > 0$, $\mu_i > \mu_e$, $\mu_e < U$ (for II_e, one should interchange the subscripts i and e), all sites are in the $|1,0\rangle$ (correspondingly $|0,1\rangle$) state. In region *III*, given by $\mu_i > U, \mu_e > U$, all sites are doubly occupied. The most interesting situation is in the neighborhood of the $\mu_i = \mu_e$ line between regions II_i and II_e, which corresponds to the half filled band, where there is a macroscopic degeneracy. We will analyze mainly this region.

After some relatively straightforward but lengthy calculations, performed partially with the aid of symbolic computation programs, we have obtained for $d = 2$ the following effective Hamiltonian up to the second order of the perturbation theory, i.e., up to terms proportional to U^{-3}:

$$H_{\Lambda,\text{eff}}^{(2)} = \left(h - 20\frac{at_{\text{ef}}^3}{U^3} \right) \sum_i s_i + \left(2\frac{t_{\text{ef}}^2}{U} - 18\frac{t_{\text{ef}}^4}{U^3} \right) \sum_{d(i,j)=1} s_i s_j$$

$$+ \frac{6t_{\text{ef}}^4 + 8a^2 t_{\text{ef}}^2}{U^3} \sum_{d(i,j)=\sqrt{2}} s_i s_j$$

$$+ \frac{4t_{\text{ef}}^4 + 2a^2 t_{\text{ef}}^2}{U^3} \sum_{d(i,j)=2} s_i s_j + \frac{8at_{\text{ef}}^3}{U^3} \sum_{S_{3,ijk}} s_i s_j s_k$$

$$+\frac{16at_{\mathrm{ef}}^3}{U^3}\sum_{\mathcal{B}_{3,ijk}}s_is_js_k+\frac{40t_{\mathrm{ef}}^4}{U^3}\sum_{\mathcal{P}_{4,ijkl}}s_is_js_ks_l$$

$$+\frac{3t_{\mathrm{ef}}^4-10a^2t_{\mathrm{ef}}^2}{2U^3}\sum_{\mathcal{P}_{4,ijkl}}1,\qquad(5)$$

where s_i is the classical one-half spin on the lattice site i; it is related to the variable w_i by the formula: $s_i=w_i-1/2$; $t_{\mathrm{ef}}=t+a$; $\mathcal{B}_{3,ijk}$—"bent" triples of spins i,j,k (i.e., the angle between bonds ij and jk is $\pi/2$); $\mathcal{S}_{3,ijk}$—"straight" triples; $\mathcal{P}_{4,ijkl}$ is a 2×2 plaquette on the lattice; $h=\mu_i-\mu_e$.

Remark 1. For $a=0$, we should obtain an effective Hamiltonian for the ordinary FKM. Comparing Eq. (5) for $a=0$ with analogous expression in Ref. 19, Table 2, we observed full consistency with the exception of the constant term [we claim that authors have omitted the term $(t^4/2U^3)P_{\{xyzw\}}^0$ (in their terminology)]. But this term is important only for absolute values of energy; it neither affects the differences of energies, nor the phase diagram.

Remark 2. The effective Hamiltonian (5) written in the spin variables corresponds to the Ising-like model with (dominating) antiferromagnetic interactions. However, there is an important aspect, as compared with the simplest FKM, that comes from the correlated hopping term (i.e., for $a\neq0$). This is the presence of terms with odd numbers of the spin operators. As a result the symmetry $h\to-h$ (present in FK and Hubbard models) no longer holds. An additional term proportional to the sum of spin variables plays a role of a supplementary external field. The other odd terms can be regarded as generalized fields.

A physical explanation of the reason why these terms with odd numbers of spin operators emerge is straightforward. Let us first focus on the linear term. Since in the chFKM the hopping rate depends on sites occupations, it is energetically favorable if all occupation numbers have one of two possible values: 1 if $a>0$ (as hopping amplitude between two occupied site is equal to $t+a$) and 0 if $a<0$. (Note that for the simplest FKM $a=0$ so the linear term does not contribute to the Hamiltonian, as it is proportional to a.) The odd terms of higher order enter in a more subtle way, as they involve three or more neighboring sites, but the principal rule stays the same: it favors an occupation number equal to 1 or 0, for $a>0$ or $a<0$, respectively.

V. THE PHASE DIAGRAM

Since there is no general method of finding ground states for classical Hamiltonians (as far as we know), we looked for the ground states of the Hamiltonian (5) by minimizing energy in some set of "trial" configurations (the method of *restricted phase diagrams*[7,8]). We took a set of all *periodic* configurations, having elementary cells up to 12 sites (there are 4000 such nonequivalent configurations), however, it appeared that *all* configurations that emerged in the phase diagram have no more than five sites per elementary cell. This observation led us to the conjection that within the assumed perturbation order our results are exact, i.e., we claim that other configurations are absent. We hope that in the future we
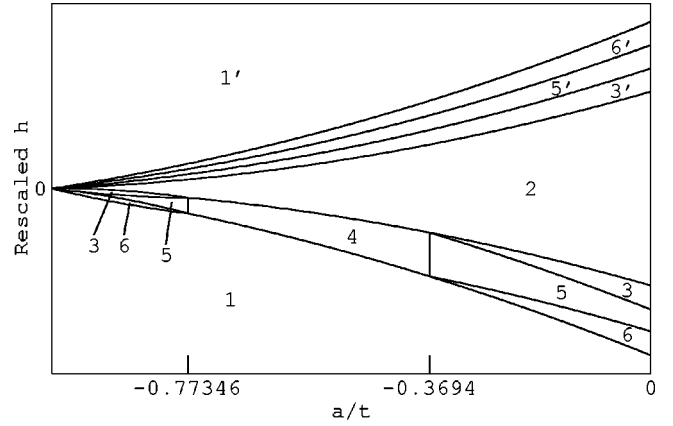

FIG. 1. Schematic phase diagram of the effective Hamiltonian (5) of the correlated hopping FKM. Phases represented by various arrangements of the ions are depicted in Fig. 2.

will be able to find a rigorous proof that our configurations are true minimizers.

The phase diagram in variables $(a/t,h)$ is displayed in Fig. 1. It can be noticed that for a predominant set of model parameters the sequence of phases agrees with that one found for the ordinary FKM (although the values of h separating subsequent phases depend strongly on a). However, it is remarkable that for $h<0$ and $a\in\,]a_-,a_+[$, where

$$a_+=(-4-\sqrt{2})/7\approx-0.773459,$$

$$a_-=(-4+\sqrt{2})/7\approx-0.369398,$$

a new type of ordering [labeled by (4)] appears, instead of the three phases (3, 5, 6). Consequently, the diagram is clearly asymmetric with respect to the horizontal axis $h=0$.

Another interesting feature of the diagram is presence of the junction point for $h=0,a=-t$, where all lines separating various phases for $h>0$, as well as most of the lines for h

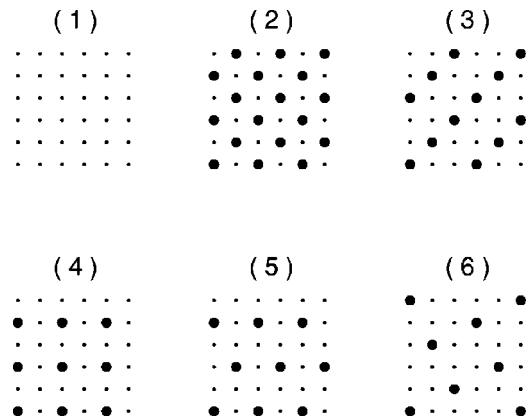FIG. 2. Configurations of the ions, marked by heavy dots ($\bullet$), corresponding to phases displayed in Fig. 1. Phases labeled by numbers with prime (e.g., $1'$, $3'$, $4'$, etc.) have mirror configurations with respect to those without prim, i.e., lattice sites occupied by the ions are then interchanged with those of unoccupied by the ions.

<0, join together. It worthwhile to notice that the exact solution has been given just for this characteristic symmetry point.[15]

VI. SUMMARY

The results obtained in this paper can be summarized as follows. First, the effective Hamiltonian of the chFKM in the second-order perturbation theory (i.e., up to terms proportional to U^{-3}) has been found, and then its ground-state phase diagram has been constructed. It has become evident from our studies that the correlated hopping term modifies substantionally the effective Hamiltonian and consequently the phase diagram of the simplest FKM. The characteristic feature of the effective Hamiltonian is the presence of odd parity terms. As the result the phase diagram becomes asymmetric with respect to the change of sign of h. In particular,

an additional ordered phase, that does not exist for the simplest FKM, has been found for a certain interval of the parameter a.

The possible directions for further studies that emerge from our results are: taking into account subsequent terms of perturbation theory, investigation the system at low, but non-zero temperatures and the inclusion of additional small terms to the quantum part of the Hamiltonian (for instance, we will allow hopping of the ions with a small amplitude $t_i \ll t_e$, thus obtaining a strongly asymmetric Hubbard model with correlated hopping).

[1] J.M. Tranquada, J. Phys. Chem. Solids **59**, 2150 (1998); H. Hwang, and S.-W. Cheong, Nature (London) **389**, 942 (1997); S. Mori, C. Chen, and S.-W. Cheong, *ibid.* **392**, 473 (1998).

[2] D. Góra, K. Rościszewski, and A.M. Oleś, Phys. Rev. B **60**, 7429 (1999); L.P. Pryadko, S.A. Kivelson, V.J. Emery, Y.E. Bazaliy, and E.A. Demler, *ibid.* **60**, 7541 (1999).

[3] L.M. Falicov, and J.C. Kimball, Phys. Rev. Lett. **22**, 997 (1969).

[4] D. I. Khomskii, in *Quantum Theory of Solids*, edited by I. M. Lifshitz (Mir, Moscow, 1982).

[5] T. Kennedy and E.H. Lieb, Physica A **138**, 320 (1986).

[6] Ch. Gruber, D. Ueltschi, and J. Jędrzejewski, J. Stat. Phys. **76**, 125 (1994).

[7] J. Lach, R. Łyżwa, and J. Jędrzejewski, Phys. Rev. B **48**, 10 783 (1993); Z. Gajek, J. Jędrzejewski, and R. Lemański, Physica A **223**, 175 (1996).

[8] G.I. Watson and R. Lemański, J. Phys.: Condens. Matter **7**, 9521 (1995).

[9] C. Gruber and N. Macris, Helv. Phys. Acta **69**, 851 (1996).

[10] K. Haller and T. Kennedy, J. Stat. Phys. **102**, 15 (2001).

[11] J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963).

[12] J.E. Hirsch, Physica C **158**, 236 (1989).

[13] K. Michielsen, Phys. Rev. B **50**, 4283 (1994); P. Farkasovsky, cond-mat/9908094 (unpublished); A. Schiller, Phys. Rev. B **60**, 15 660 (1999); K. Michielsen and H. de Raedt, *ibid.* **59**, 4565 (1999).

[14] A.A. Aligi, L. Arrachea, and E.R. Gagliano, Phys. Rev. B **51**, 13 774 (1995); J.C. Amadon and J.E. Hirsch, *ibid.* **54**, 6364 (1996); L. Didukh, V. Hankevych, and Yu. Skorenkyy, Physica B **284-288**, 1537 (2000); M. Kollar and D. Vollhardt, Phys. Rev. B **63**, 045107 (2001).

[15] R. Strack and D. Vollhardt, Phys. Rev. Lett. **70**, 2637 (1993).

[16] N. Datta, R. Fernandez, and J. Fröhlich, J. Stat. Phys. **84**, 455 (1996).

[17] N. Datta, L. Rey-Bellet, J. Fröhlich, and R. Fernandez, Helv. Phys. Acta **69**, 752 (1996).

[18] J. Fröhlich, and L. Rey-Bellet, Helv. Phys. Acta **69**, 821 (1996).

[19] N. Datta, R. Fernandez, and J. Fröhlich, J. Stat. Phys. **96**, 545 (1999).

[20] S.A. Pirogov and Ya.G. Sinai, Teor. Mat. Fiz. **25**, 358 (1975); **26**, 61 (1976).

[21] Ch. Gruber, N. Macris, A. Messager, and D. Ueltschi, J. Stat. Phys. **86**, 57 (1997).

[22] T. Kennedy, Rev. Math. Phys. **6**, 901 (1994).

[23] J. Slawny, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz (Academic Press, London/New York, 1985), Vol. 11.

[24] C. Borgs, R. Kotecky, and D. Ueltschi, Commun. Math. Phys. **181**, 409 (1996); R. Kotecky and D. Ueltschi, *ibid.* **206**, 289 (1999); C. Borgs and R. Kotecky, *ibid.* **208**, 575 (2000).

[25] Ch. Gruber, R. Kotecky, and D. Ueltschi, J. Phys. A **33**, 7857 (2000).