LOW TEMPERATURE STATES IN THE FALICOV-KIMBALL MODEL

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Abstract: The ground states and low temperature states of the Falicov-Kimball model are studied in the plane of chemical potentials of the two sort of particles involved, for large values of the coupling constant, near the half filled band. For this study, a cluster expansion is introduced which can be used to investigate the effective interaction energy between the static particles.

1. Introduction

The Falicov-Kimball model [1] is one of the simplest lattice systems of interacting fermions. It consists of spinless Fermi particles, which we refer to as electrons, and classical particles, which we refer to as nuclei. The electrons can hop between nearest neighbour sites and there is an on-site interaction between electrons and nuclei. At most one nucleus is allowed at each lattice site. Let the system be in a finite box Λ of a d-dimensional regular lattice. The hamiltonian is

$$H_\Lambda = -k \sum_{(x,y)\subset\Lambda} c^+(x)c(y) + 2U \sum_{x\in\Lambda} w(x)c^+(x)c(x)$$

where $c^+(x)$, $c(x)$ are the creation and annihilation operators for electrons at site x. The first sum runs over ordered pairs of nearest neighbour sites and $k > 0$ is the hopping coefficient (the usual notation t for the hopping coefficient will be reserved here to indicate the "time" variable in the path integral representation of the system). The variable $w(x)$ is 1 or 0 according to whether the site x is occupied or non-occupied by a nucleus. It will be convenient to introduce, also, the spin variables $s(x) = 2w(x) - 1$ ($s(x) = \pm 1$), to describe the nuclei configurations. The total number of electrons and nuclei are

$$N_e = \sum_{x\in\Lambda} c^+(x)c(x)\ , \qquad N_n = \sum_{x\in\Lambda} w(x)$$

The above description, in which the system is considered as a very simplified model for mater, is only one of the possible interpretations. This interpretation was used in Ref. 2 to study the crystallization effect. Falicov and Kimball introduced this model to study semiconductor-metal transitions in solids. The model can also be interpreted as a simplified version of the Hubbard model, in which one of the particles is infinitely massive and cannot hop. In the last two contexts one takes $U > 0$. Although we are following the first interpretation, for which $U < 0$ would be more appropriate, we shall consider also that $U > 0$. Due to the symmetries of the model, both cases, $U > 0$ and $U < 0$, are mathematically equivalent. Notice, however, that the half filled condition, which plays a particular role in the case $U > 0$ and says that

$$\rho_e + \rho_n = 1$$

where ρ_e and ρ_n are, respectively, the densities of the electrons and the nuclei, corresponds to the neutrality condition

$$\rho_e = \rho_n$$

in the case $U < 0$. We remark that, as a consequence of the exclusion principle, $0 \leq \rho_e + \rho_n \leq 2$.

In a first rigorous study of the model, Kennedy and Lieb [2] proved that the ground state occurs in the half filled band and that the nuclei are antiferromagnetically ordered. It is assumed that $\mathcal{L}$ is a bipartite lattice, that is, that the lattice $\mathcal{L}$ may be broken up into two sublattices $\mathcal{L}_1$ and $\mathcal{L}_2$ with the property that all nearest neighbours of a site on the sublattice $\mathcal{L}_1$ belong to the sublattice $\mathcal{L}_2$ and viceversa. They proved also that the antiferromagnetic long range order continues to exist at low temperatures. These results are valid for any $U > 0$.

In the present work we study the Falicov-Kimball model for U sufficiently large, at low temperatures. We consider the grand canonical ensemble, specified by the density matrix

$$\rho = Z(\Lambda)^{-1} \exp\big(-\beta(H_\Lambda - \mu_e N_e - \mu_n N_n)\big)$$

with the partition function defined as

$$Z(\Lambda) = Z(\Lambda, \beta, \mu_e, \mu_n) = \sum_{\{w(x)\}} \mathrm{Tr}\; e^{-\beta(H_\Lambda - \mu_e N_e - \mu_n N_n)}$$

Here β is the inverse temperature and μ_e, μ_n are the electron and nucleus chemical potentials. The sum is over all nuclei configurations, with appropriate boundary conditions, and the trace is over the electron Fock space.

We shall concentrate on the nuclei subsystem. We observe that since the only interaction is on-site, neither the potential energy nor the kinetic energy alone can produce long range order in the system. If the nuclei exhibit long range order it must come about because the interplay between both terms of the hamiltonian produce an effective interaction between the nuclei.

This effective interaction energy can be defined by means of the grand canonical partition function

$$Z(\Lambda)=\sum_{\{s(x)\}}\mathrm{Tr}\ e^{-\beta(H_\Lambda-\mu_e N_e-\mu_n N_n)}=\sum_{\{s(x)\}}\exp\big(-\beta G_\Lambda(s)\big)$$

We shall rigorously determine the effective interaction energy $G_\Lambda(s)$ with the help of a cluster expansion. This expansion follows from the Feynman-Kac or path integral representation of the system. Provided that the electron chemical potential is such that $|\mu_e - U|$ is bounded, we prove that the cluster expansion, in powers of $1/U$, is absolutely convergent for large U. Namely, under the condition

$$U-|\mu_e-U|>2d(1+C_0)k$$

where $C_0>0$ is a given number (not a large constant). There is no restriction on the chemical potential μ_n. The effective interaction properly describes the nuclei subsystem if the temperature is low enough (i. e., if $\beta>\beta_0$, where β_0 is some constant). All these constants are independent of $|\Lambda|$, the size of the system.

It is shown that the cluster expansion gives the effective hamiltonian in terms of usual interaction potentials

$$G_\Lambda(s)=\sum_{A\subset\Lambda}\Phi_A(s_A)$$

where $A=\{x_1,\dots,x_n\}$ are finite sets of sites, and $s_A=\{s(x_1),\dots,s(x_n)\}$ is the restriction to A of the configuration s. The interaction potentials are translation invariant.

The main contributions to the Φ_A are independent of the temperature and the chemical potentials. The small contributions, which depend on β and μ_e, can be grouped in a term $\tilde\Phi_A$ of order $e^{-\beta U}$.

The cluster expansion allows us (in principle) to compute the potentials $\Phi_A(s_A)$ at all orders. We remark that $\Phi_A\neq 0$ only if A is a connected set of sites (by paths going along nearest neighbours). Moreover, $\Phi_A(s_A)$ is of order U^{-n}, where n is the minimum number of bonds visited by a closed path which passes through all sites of A.

The correlation functions between the nuclei can be expressed as the associated classical correlations with respect to the hamiltonian $G_\Lambda(s)$ This will be clear from the discussion in Section 2 (an expression in terms of the objects considered in the cluster expansion can also be found for the quantum correlations, or reduced density matrices). Therefore, if the convergence conditions of the cluster expansion are satisfied, the study of the nuclei subsystem in the Falicov-Kimball model, is reduced to a classical lattice system problem. Moreover, when a given approximation is considered, one has, by means of the cluster expansion, a full control on the terms neglected in the interaction, at any order.

For example, let us consider the first terms of the effective interaction energy. One finds

$$G_\Lambda^{(1)}(s)=-\frac{1}{2}(\mu_n-\mu_e)\sum_x s(x)+\frac{k^2}{4U}\sum_{(x,y)}s(x)s(y)$$

Then, up to the order U^{-1}, the situation appears to be near to that of the Ising model with nearest neighbour antiferromagnetic interactions in the presence of a external magnetic field. For the cubic lattice $\mathcal{L} = \mathbb{Z}^d$, with $d \geq 2$ (and, more generally, for a bipartite lattice), we find, as Lebowitz and Macris [3], that a long range order of chess board type exist, for the nuclei, at low enough temperatures. The system presents the two corresponding phases. This happens (for $d = 2$) provided that the chemical potentials satisfy $\frac{1}{2}|\mu_n - \mu_e| < k^2 U^{-1} - \eta$, where η is some positive quantity of order U^{-3}. As noticed in Ref. 3 the system is not exactly in the half filled band at positive temperature, unless $\mu_e - U = 0$. This comes from the presence of the terms $\tilde{\Phi}_A$ in the hamiltonian. Nevertheless, the half filled condition holds exactly in the limit $\beta \to \infty$, with the positions of the nuclei forming a perfect chess board configuration.

Computing the next terms in the interaction potentials, up to order U^{-3}, we find, for a cubic lattice $\mathcal{L} = \mathbb{Z}^d$, with $d \geq 2$, the approximate hamiltonian denoted $G_\Lambda^{(3)}(s)$, whose expression is given in Section 3. This expression agrees with the formula, for the ground state energy, up to order U^{-3}, given by Gruber *et al.*, on the basis of a non rigorous perturbation theory [4,5]. The ground state configurations associated to this hamiltonian, in the case of the square lattice ($d = 2$), have also been examined in Ref. 5. Besides the chess board configurations of density $\rho_n = 1/2$, three other kinds of periodic ground configurations, which correspond to the densities $\rho_n = 1/3$, $1/4$ and $1/5$, are found, for different specified values of the chemical potentials. We notice that Kennedy [6] has rigorously justified the existence of these periodic ground configurations, when U is sufficiently large, in a recent study of the ground states of this model at fixed densities. This study includes also several results concerning the system outside the half filled band.

We prove that the ground state configurations of the nuclei subsystem, in the Falicov-Kimball model, coincide with the above periodic configurations (for U sufficiently large and suitable values of μ_e). We describe, also, the corresponding phase diagram in terms of the variable $h = (1/2)(\mu_n - \mu_e)$. The different domains where the configurations of densities $\rho_n = 1/3$, $1/4$ and $1/5$ are proved to be the periodic ground states, have lengths of order U^{-3} and are situated around the point $h = -k^2 U^{-1}$. These domains are separated, between them and from the domain where the chess board configurations are the ground states, by small intervals whose length is of order U^{-5}. In order to investigate the gound state phase diagram inside these small intervals the next order terms in the nuceli effective interaction have to be considered.

On the other side, we expect that Gibbs states exist, at sufficiently low temperatures, that are near, in some sense, to the periodic ground states described above, for every h in the corresponding domain of the ground state phase diagram (see the discussion at the end of Section 3). We finally remark that extensions of the present study to other kinds of lattices are possible along the same lines.

2. A cluster expansion

In this Section we analyse the Feynman-Kac or path integral representation of the model. This representation is discussed in Appendix 1 in a more general context. As a consequence of this analysis we shall see that, under appropriate conditions, the model admits a convergent cluster expansion which can be related to the effective interaction energy between the nuclei.

We consider the model to be defined on a finite d-dimensional cubic lattice $\Lambda \subset \mathbb{Z}^d$. Nevertheless, the discussion below can be applied in a similar way to other kinds of regular lattices. Let us denote by $Q(\Lambda) = \{-1, 1\}^\Lambda$ the set of nuclei configurations. Given $s \in Q(\Lambda)$, the sites where $s(x) = 1$ correspond to the sites occupied by a nucleus. Including the inverse temperature factor β in the coupling constants of the hamiltonian, the partition function is defined as follows

$$Z(\Lambda) = \sum_{s \in Q(\Lambda)} Z(\Lambda, s) = \sum_{s \in Q(\Lambda)} \operatorname{Tr} \exp(-H_\Lambda + \mu_n N_n + \mu_e N_e)$$

In Appendix 1, an expression is given of this partition function in terms of oriented circuits. ¿From the discussion it may be seen that, also, the correlation functions associated to the nuclei subsystem admit a representation in terms of the same objects. The oriented circuits, whose precise definition is given in Appendix 1, belong, as geometric objects, to a finite cubic lattice Ω^{per} of $d + 1$ dimensions. A site $\xi \in \Omega^{\text{per}}$, is a couple (x, t), where $x \in \Lambda$ and $t \in \{0, 1, \ldots, T\}$. The lines in the direction of the t variable (the "time") are called vertical lines. The two horizontal faces of Ω^{per}, corresponding to $t = 0$ and $t = T$, are identified (periodic boundary conditions in time). In all this study, the discrete time Feynman-Kac representation is used in order to simplify the notations. The passage to the continuous time representation, obtained in the limit $T \to \infty$, does not present any special difficulty (see, for instance, Ref. 7).

The following expression for the partition function (last formula in Appendix 1) is found

$$Z(\Lambda, s) = \lim_{T \to \infty} \sum_{\{\omega_1, \ldots, \omega_r\}} \prod_{q=1}^{r} \exp(-\frac{\lambda(\omega_q)}{T}) \left(\frac{k}{T}\right)^{j(\omega_q)} \alpha(\omega_q)$$

In this formula the sum is over all compatible families of oriented dashed circuits $\{\omega_1, \ldots, \omega_r\}$, $r = 0, 1, \ldots$, which, moreover, are compatible with the configuration $s \in Q(\Lambda)$. The factor $\alpha(\omega_q)$, equal to $+1$ or -1, is a sign associated with the circuit (coming from the anticommutation relations), $j(\omega)$ is the number of jumps of the circuit ω, and $\lambda(\omega)$ is a function of ω related to the potential energy. In order to show a different point of view, the analysis in Appendix 1 is developed in the canonical ensemble for the half filled band, i. e., in the canonical ensemble where the total number of particles is $N = |\Lambda|$. In this case $\lambda(\omega) = U|\omega|$, where $|\omega|$ is the length of the circuit. This expression has to be modified in order to include the chemical potentials μ_n and μ_e.

Consider a vertical bond $b = [(x, t), (x, t + 1)] \in \Omega^{\text{per}}$ and a given circuit configuration in Ω^{per}, compatible with the given classical configuration $s \in \Lambda$. As explained in Appendix 1 four situations, called there cases (1) to (4), can occur.

According with the compatibility conditions between the circuits configuration and the classical configuration $s \in Q(\Lambda)$, we have: $s(x) = 1$ in cases (1) and (3) and, $s(x) = -1$ in cases (2) and (4). Taking into account the chemical potentials, the contribution to the potential energy, of the bond $b \in \Omega^{\text{per}}$, is

$$\begin{aligned}
\mu_n &= \frac{1}{2}(\mu_n + \mu_e) + \frac{1}{2}(\mu_n - \mu_e)s(x) && \text{in case (1)},\\
\mu_e &= \frac{1}{2}(\mu_n + \mu_e) + \frac{1}{2}(\mu_n - \mu_e)s(x) && \text{in case (2)},\\
\mu_n + \mu_e - 2U &= \frac{1}{2}(\mu_n + \mu_e) + \frac{1}{2}(\mu_n - \mu_e)s(x) + \mu_e - 2U && \text{in case (3)},\\
0 &= \frac{1}{2}(\mu_n + \mu_e) + \frac{1}{2}(\mu_n - \mu_e)s(x) - \mu_e && \text{in case (4)}.
\end{aligned}$$

Therefore, if we write

$$Z(\Lambda, s) = \exp\Big[\frac{1}{2}(\mu_n + \mu_e)|\Lambda| + \frac{1}{2}(\mu_n - \mu_e)\sum_{x\in\Lambda} s(x)\Big]\ \tilde{Z}(\Lambda, s)$$

it appears that there is no weight associated to the oriented continuous circuits in $\tilde{Z}(\Lambda, s)$. This partition function can be written using only the oriented dashed circuits, and we have

$$\tilde{Z}(\Lambda, s) = \lim_{T\to\infty} \sum_{\{\omega_1,\ldots,\omega_r\}} \prod_{q=1}^{r} \exp\Big(-\frac{\lambda(\omega_q)}{T}\Big)\left(\frac{k}{T}\right)^{j(\omega_q)} \alpha(\omega_q)$$

If ω is a circuit which does not wind around the cylinder Ω^{per}, the number of vertical unit segments with up arrows, case (3), coincides with the number of vertical unit segments with down arrows, case (4). For such a circuit, we have

$$\lambda(\omega) = U|\omega|$$

where $|\omega|$ is the length of ω (i. e., the number of vertical unit segments of ω). If ω is a circuit which goes around the cylinder Ω^{per} (i. e., has a winding number $\neq 0$), then ω can be decomposed into connected paths which can be said to belong to two different classes. For the paths of the first class, the above property still holds. For the paths of the second class, either, all vertical unit segments of the path have up arrows (for circuits which wind around the cylinder in the positive sense), or, all of them have down arrows (for circuits which wind around the cylinder in the negative sense). Let $\ell_1(\omega)$ and $\ell_2(\omega)$ be the total lengths of the paths belonging to the first and to the second class, respectively. Then,

$$\lambda(\omega) = U\ell_1(\omega) - (\mu_e - 2U)\ell_2(\omega)$$

for the circuits going in the positive sense, and

$$\lambda(\omega) = U\ell_1(\omega) + \mu_e\ell_2(\omega)$$

for the circuits going in the negative sense.

Let ω be an oriented dashed circuit. We define the activity of ω, with respect to the specified classical configuration $s \in Q(\Lambda)$, by

$$\varphi_s(\omega) = \exp\left(-\frac{\lambda(\omega)}{T}\right)\left(-\frac{k}{T}\right)^{j(\omega)} \alpha(\omega)$$

if ω is compatible with s (i. e., if its vertical segments have the orientation specified by s), and by

$$\varphi_s(\omega) = 0$$

otherwise. Two oriented dashed circuits, compatible with the same configuration s, are mutually compatible if, and only if, they do not intersect. We say that any set of pair wise disjoint oriented dashed circuits is an admissible family of circuits. Then,

$$\tilde{Z}(\Lambda, s) = \lim_{T\to\infty} \sum_{\theta\subset\Omega^{\rm per}} \prod_{\omega\in\theta} \varphi_s(\omega)$$

where the sum runs over all admissible families of oriented dashed circuits inside $\Omega^{\rm per}$.

This expression shows that the system of dashed circuits is equivalent to a polymer system, i.e., to a gas of several "species of particles" (all dashed circuits), interacting only through hard-core exclusion and having the (non translation invariant) activity $\varphi_s(\omega)$. The properties of polymer systems at low activities may, under appropriate conditions, be studied with the help of convergent expansions. We shall use the theory of these expansions presented in Refs. 8 and 9.

For this purpose, consider also non-admissible families of oriented dashed circuits, including families in which a circuit occurs several times. They are identified with the non-negative integer valued functions θ on the set of oriented dashed circuits such that $\sum_\omega \theta(\omega) < \infty$, where $\theta(\omega)$ is the multiplicity of the circuit ω in the family. Let $\mathcal{M}$ be the set of all these multiplicity functions, and define $(\theta_1 + \theta_2)(\omega) = \theta_1(\omega) + \theta_2(\omega)$. We shall also use the notation θ, for $\omega_1 \cup ... \cup \omega_r$, considered as a set in $I\!R^d$, where $\omega_1, ..., \omega_r$ are all the circuits for which $\theta(\omega_i) \neq 0$. Moreover, the length of a cluster θ is defined by $|\theta| = |\omega_1| + \ldots + |\omega_r|$, and the total number of jumps in θ by $j(\theta) = j(\omega_1) + \ldots + j(\omega_r)$.

One extends the Boltzmann factor to $\mathcal{M}$ by putting $\varphi_s(\theta) = \prod_{\omega\in\theta} \varphi_s(\omega)$, if θ is admissible, and $\varphi_s(\theta) = 0$, otherwise. One defines on $\mathcal{M}$ the truncated functions, $\varphi_s^{\rm C}$, by

$$\varphi_s^{\rm C}(\theta) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sum{}' \prod_{i=1}^{n} \varphi_s(\theta_i)$$

where the sum $\sum'$ is over all $\theta_1, ..., \theta_n$ such that $\theta_i \neq \emptyset$ for all $i = 1, \ldots, n$ and $\sum \theta_i = \theta$.

A first consequence of this definition is that if $\varphi_s^{\rm C}(\theta) \neq 0$ then θ is connected as a set in $I\!R^d$. A second consequence is that

$$\tilde{Z}(\Lambda, s) = \lim_{T\to\infty} \exp(\sum_{\theta\subset\Omega} \varphi_s^{\rm C}(\theta))$$

The connected θ will be called clusters (of oriented dashed circuits). The expansions in terms of the functions $\varphi_s^{\rm C}(\theta)$ are the cluster expansions.

It is convenient to define the functions $\varphi_s^{\mathrm{C}}(\theta)$ for clusters and circuits of any size. For this purpose we shall now consider the lattice Ω^{per}, infinitely extended in the spatial directions, $\Lambda \to \mathbb{Z}^d$, but with unchanged dimension in the time direction, and the classical nuclei configurations, as given configurations $s \in Q(\mathbb{Z}^d)$ on the infinite lattice $\mathbb{Z}^d$.

For any cluster θ, let $\pi(\theta) \subset \mathbb{Z}^d$ be the set of sites which belong to the horizontal projections of all vertical lines of θ (i.e., all vertical lines of the circuits ω for which $\theta(\omega) \neq 0$). The set $\pi(\theta)$ is finite. Since the vertical lines in θ are connected by jumps, it follows that $\pi(\theta)$ is connected (in the sense that the sites in $\pi(\theta)$ are connected by the bonds which join nearest neighbour sites).

Let a site $x \in \Lambda$ be given, and consider the series

$$F_x(s) = \sum_{\theta : x \in \pi(\theta)} \varphi_s^{\mathrm{C}}(\theta)$$

It will be shown that the series $F_x(s)$ is absolutely convergent, provided that U is sufficiently large and that μ_e varies in some specified interval. The precise conditions will be given below.

We first prove that, for any $\xi \in \Omega^{\mathrm{per}}$, and under the appropriate conditions, the series

$$\sum_{\omega : \xi \in \omega} \varphi_\sigma(\omega)$$

is absolutely convergent. We begin by considering the restriction of this sum to non-winding circuits. As explained in Appendix 1, such a circuit is described by the set of its vertices $\xi_0, \xi_1, \ldots, \xi_{2l} = \xi_0$, satisfying some conditions, with $\xi_q = (x_q, t_q) \in \Omega^{\mathrm{per}}$. Let $(\xi_0, \xi_1), (\xi_2, \xi_3), \ldots, (\xi_{2l-2}, \xi_{2l-1})$ be the vertical lines of ω, of lengths $m_i = |t_{2i-1} - t_{2i-2}|$, $i = 1, 2, ..., l$. Let $(\xi_1, \xi_2), (\xi_3, \xi_4), \ldots, (\xi_{2l-1}, \xi_{2l})$ be the l horizontal segments. Assume that in our notations the first vertical line (ξ_0, ξ_1) of ω passes through the point $\xi = (x, t) \in \Omega^{\mathrm{per}}$ (i.e., $x = x_0 = x_1$ and $t_0 \le t \le t_1$), and let $m_1' = |t - t_0|$ and $m_1'' = |t_1 - t|$. The length of the circuit is

$$|\omega| = \frac{1}{2}(m_1 + m_2 + \ldots + m_l) \ge \frac{1}{2}(m_1' + m_1'' + m_2 + \ldots + m_{l-1})$$

Once the l positive integers $m_1', m_1'', m_2, \ldots, m_{l-1}$ are given, we have still,in order to determine the circuit, the choice of the directions of the l horizontal segments. These choices give at most $(2d)^l$ possibilities. As a consequence of these facts, we obtain

$$\begin{aligned}
\sum_{\xi \in \omega} |\varphi_s(\omega)| &= \sum_{\xi \in \omega} e^{-\frac{U}{T}|\omega|} (\frac{k}{T})^{j(\omega)} \\
&\le \sum_{l \ge 2} \frac{1}{T^l} \sum_{m_1', \ldots, m_{l-1}} e^{-\frac{U}{T}(m_1' + m_1'' + m_2 + \ldots + m_{l-1})} \, (2d)^l k^l \\
&\le \sum_{l \ge 2} \Big(\frac{1}{T} \sum_{m \ge 0} \exp(-\frac{U}{T} m) \Big)^l (2dk)^l
\end{aligned}$$

and, because

$$\frac{1}{T}\sum_{m\geq 0}\exp(-\frac{U}{T}m) = T^{-1}(1-e^{-(U/T)})^{-1} \longrightarrow_{T\to\infty} 1/U$$

it follows that the sum converges if $U > 2dk$. More precisely, if $Uk^{-1} \geq 2d(1+a_1)$, where $a_1 > 0$ is any chosen constant, then the sum converges for all $T > T_0$, where $T_0(U, a_1)$ is some constant (which depends on U and a_1).

Let us now discuss the case in which the circuits winding around the cylinder Ω^{per} are included in the sum. Except for the circuit with zero jumps (which can be treated apart), the argument above can be extended to the winding circuits, provided that one takes into account that some of the vertical segments of length m_q will get, instead of the weight $\exp(-(U/T)m_q)$, either the weight $\exp((\mu_e-2U)/T)m_q$, when ω goes around Ω^{per} in the positive sense, or the weight $\exp(-(\mu_e/T)m_q)$, when ω goes around Ω^{per} in the negative sense. By writing $\mu_e - 2U = -U + (\mu_e - U)$ and $-\mu_e = -U - (\mu_e - U)$, we see that the sum converges if the inequality $U - |\mu_e - U| > 2dk$ is satisfied. Or, more precisely, if $U - |\mu_e - U| \geq 2d(1+a_1)k$, for some $a_1 > 0$, then, the sum converges for all $T > T_0(U, a_1)$. As a consequence of these facts and of the general theory of cluster expansions, whose application to the present case is explained in Appendix 2, the following result follows.

Theorem 1. *There exists a positive constant C_0, such that, if*

$$U - |\mu_e - U| \geq 2d(1+C_0)k$$

then, the series in the definition of the function $F_x(s)$ is absolutely convergent.

We notice that C_0 is a number which can be computed from the theory (it is not a large constant). We notice, also, that the convergence condition is independent of the number T of time intervals. The stated results hold uniformly for all $T > T_0(U, a_1)$. This allows us to pass to the limit $T \to \infty$ and recover the continuous time expressions in terms of path integrals. On the other side the absolute convergence of the series $F_x(s)$, as well as all the estimates which have been used, hold uniformly for all configurations $s \in Q(\Lambda)$.

We, finally, comment on the convergence condition. Clearly, it is needed that $U > |\mu_e - U|$. Let η be defined by $\eta U = \mu_e - U$. Then the inequalities $|\eta| < 1$ and $U(1-|\eta|) \geq 2d(1+C_0)k$ are required. If one takes $\eta = 0$, or equivalently $\mu_e = U$, then the best value for U is obtained. This choice gives the same weight to both kinds of winding circuits, those going around Ω^{per} in the positive sense, and those going in the negative sense. The system described by the grand canonical ensemble is, with probability near to one, in the half filled band. If $\eta \neq 0$ the two kinds of winding circuits have different weights, and the half filled condition is not exactly satisfied. However, it may be seen, though this fact was not used in the above estimates, that the winding circuits, whose length is always at least equal to the number T of time intervals, have a very small weight (provided, naturally, that the convergence condition is satisfied). The density of the clusters with winding circuits tends exponentially to zero when U (or β) becomes large, and the system comes near to the half filled band.

3. The effective interaction energy. Properties and consequences.

In Section 2 an expression has been found for the effective interaction energy which describes the nuclei subsystem in the Falicov-Kimball model. The validity of this description, with appropriate assumptions, has been justified by means of the cluster expansion discussed in that Section. In the present Section we want to investigate further properties of the effective interaction. As a consequence of this analysis, a number of results concerning the low temperature states of the system will be derived.

Let us recall, from Section 2, that the partition function is

$$Z(\Lambda) = \sum_{s\in Q(\Lambda)} \mathrm{Tr}\; e^{-H_\Lambda+\mu_e N_e+\mu_n N_n} = e^{\frac{1}{2}(\mu_n+\mu_e)|\Lambda|} \sum_{s\in Q(\Lambda)} e^{-G_\Lambda(s)}$$

where, the effective interaction energy is given by

$$G_\Lambda(s) = -\frac{1}{2}(\mu_n-\mu_e)\sum_{x\in\Lambda} s(x) - \sum_{\theta\subset\Omega^{\mathrm{per}}} \varphi_s^C(\theta)$$

The last sum is over the clusters θ, of oriented dashed circuits, contained in the $(d+1)$-dimensional cylinder lattice Ω^{per}, and φ_s^C are the truncated functions associated with the classical configuration $s \in Q(\Lambda)$ (i. e., the oriented circuits in the cluster θ are compatible with the configuration s). The correlation functions of the nuclei subsystem can also be expressed as classical correlation functions with respect to the hamiltonian $G_\Lambda(s)$.

The formula above gives the hamiltonian $G_\Lambda(s)$ in terms of usual interaction potentials

$$G_\Lambda(s) = \sum_{A\subset\Lambda} \Phi_A(s_A)$$

where $A = \{x_1,\ldots,x_n\}$ are finite sets of sites and $s_A = \{s(x_1),\ldots,s(x_n)\}$ is the restriction to A of the configuration $s \in Q(\Lambda)$. Moreover, the interaction potentials $\Phi_A(s_A)$ are translation invariant. To see these facts, we recall the notion of horizontal projection $\pi(\theta)$ of a cluster θ, introduced in Section 2. Then

$$\Phi_A(s_A) = \lim_{T\to\infty} \sum_{\theta:\pi(\theta)=A} \varphi_s^C(\theta)$$

where the condition $\theta \subset \Omega^{\mathrm{per}}$ is understood. It is clear that, for $\pi(\theta) = A$, the functions $\varphi_s^C(\theta)$ depend only on the restriction s_A of the configuration s.

It will be useful to consider the perturbative expansion of the interaction potentials obtained by taking into account the total number of jumps of the clusters $j(\theta)$ (see Section 2 for the definition). The component of order n of the potential is defined by

$$\Phi_A^{(n)}(s_A) = \lim_{T\to\infty} \sum_{\substack{\theta:\pi(\theta)=A \\ j(\theta)=n}} \varphi_s^C(\theta)$$

and, we have

$$\Phi_A(s_A) = \sum_{n\geq 0} \Phi_A^{(n)}(s_A)$$

¿From the discussion in Section 2, it follows that $\Phi_A \neq 0$, only if A is a connected set of sites (in the sense that A with the bonds joining the nearest neighbours is a connected graph). Since the number of jumps $j(\theta)$, is always even (in a cubic lattice), their contribution to $\Phi_A^{(n)}$ is $\neq 0$, only if n is an even number. Moreover, $\Phi_A^{(n)} \neq 0$, only if n is larger or equal than the smallest length (number of bonds) which can have a closed path, along the bonds of A, which passes through all sites of A. It is also convenient to distinguish the contributions to $\Phi_A^{(n)}$ which come from clusters made only with non-winding circuits, from the contributions of clusters in which at least one of its circuits is winding around the cylinder Ω^{per}. We denote by $\tilde{\Phi}_A^{(n)}$ the last mentioned contributions to $\Phi_A^{(n)}$.

Next, we examine a first example. The simplest cluster is the cluster which reduces to one non-winding circuit with two jumps (see Fig. 1). Such a circuit, say ω, is a rectangle with horizontal sides of length 1, and vertical sides of length m $(1 \leq m \leq T)$, in which some orientation is given. It projects on a pair of nearest neighbour sites, (i. e., $\pi(\omega) = \{x, y\}$ with $|x-y| = 1$). It can exits (as an oriented circuit) if, and only if, $s(x) = -s(y)$, and, in this case,

$$\varphi_s^C(\omega) = \varphi_s(\omega) = e^{-\frac{2U}{T}m}(k/T)^2\alpha(\omega)$$

with $\alpha(\omega) = 1$. Therefore, if $s(x) = -s(y)$, we get

$$\Phi_{\{x,y\}}^{(2)}(s(x), s(y)) = \lim_{T\to\infty} T \sum_{m=1}^{T} e^{-\frac{2U}{T}m}(\frac{k}{T})^2 = \frac{k^2}{2U}(1 - e^{-2U})$$

Let us assume, for a moment, that this is the largest contribution to the effective interaction energy when U is large. If all other contributions are neglected (and also the terms of order e^{-2U}), one obtains

$$G_\Lambda^{(1)}(s) = -\frac{1}{2}(\mu_n - \mu_e)\sum_{x\in\Lambda} s(x) + \frac{k^2}{4U}\sum_{|x-y|=1} \big(s(x)s(y) - 1\big)$$

That is, one obtains the hamiltonian of the Ising model with nearest neighbour antiferromagnetic interactions and an external magnetic field. We are going to show that, in fact, this model is not so far from the system under consideration. Provided that the appropriated conditions (which will be made precise below) are satisfied, the nuclei, in the Falicov-Kimball model, present a long range order of antiferromagnetic type at low temperatures.

For this purpose let us first consider the class of circuits winding around the cylinder $\Omega^{\rm per}$ and having zero or two jumps. In order to simplify the exposition, we choose $\mu_e = U$. There is no difficulty, however, in treating the general case, considered in the convergence condition of Theorem 1 (see the remarks in the last paragraph of Section 2).

There is a cluster which consists only of a circuit with zero jumps, it is just the oriented vertical line from $t = 0$ to T, which may lie above any site $x \in \Lambda$. The contribution of this cluster is

$$\tilde{\Phi}^{(0)}_{\{x\}} = e^{-\frac{U}{T}T} = e^{-U}$$

in both cases, $s(x) = 1$ or $s(x) = -1$. It adds a constant term $|\Lambda| e^{-2U}$ to the hamiltonian $G_\Lambda(s)$. Oriented winding circuits with two jumps can be constructed above any pair of nearest neighbour sites $\{x, y\}$ provided that $s(x) = s(y)$. The contribution of the clusters which consist only of one of these circuits is

$$\tilde{\Phi}^{(2)}_{\{x,y\}} = \lim_{T\to\infty} e^{-\frac{U}{T}T} \binom{T}{2} \frac{k^2}{T^2} = \frac{k^2}{2} e^{-U}$$

when $s(x) = s(y)$ (the combinatorial factor $\binom{T}{2}$ gives the number of possible choices for the jumps).

The next step is to estimate the contributions of the clusters with more than two jumps. Let θ be a given cluster, with $n = j(\theta)$ jumps, compatible with the configuration $s \in Q(\Lambda)$. Assume that the jumps occur at times $t_1 \le t_2 \le \ldots \le t_n$ and write $m_1 = t_2 - t_1, \ldots, m_{n-1} = t_n - t_{n-1}$. Define the family of clusters $\mathcal{F}(\theta)$, which have the same shape than θ, by varying the integers $m_1, \ldots, m_{n-1}$ (restricted only by the constraints $m_1 \ge 1, \ldots, m_{n-1} \ge 1$ and $m_1 + \ldots + m_{n-1} \le T$), and letting the initial time t_1 to take all values $t_1 = 1, 2, \ldots, T$. The periodicity of $\Omega^{\rm per}$ in the time direction is used in this definition. It is clear that all clusters in the family $\mathcal{F}(\theta)$ are compatible with the configuration $s \in Q(\Lambda)$. On the other side, there is a finite number of possible cluster shapes for any n.

Consider first the case in which all circuits in the cluster θ are non-winding circuits, and let $q_l(\theta)$ be the number of vertical lines in θ between the times t_l and t_{l+1} (for $l = 1, \ldots, n-1$). The contribution to $G_\Lambda(s)$ of all clusters in the family $\mathcal{F}(\theta)$ can be written (assuming the following sums to be restricted to the admissible values of $m_1, \ldots, m_{n-1}$ mentioned above),

$$T \sum_{m_1,\ldots,m_{n-1}} e^{-\frac{U}{T}\left((m_1 q_1(\theta) + \ldots + m_{n-1} q_{n-1}(\theta)\right)} \left(\frac{k}{T}\right)^n$$
$$= k \left(\frac{k}{U}\right)^{n-1} \sum_{m_1,\ldots,m_{n-1}} \left(\frac{U}{T}\right)^{n-1} e^{-\left(q_1(\theta)\frac{Um_1}{T} + \ldots + q_{n-1}(\theta)\frac{Um_{n-1}}{T}\right)}$$

We remark that the last sum has the form of a Riemann sum, it has therefore a limit when $T \to \infty$, which gives the corresponding integral. The same occurs when θ contains winding circuits. The difference is only that, in this case, the factor $\exp\big(-\frac{U}{T}(\nu(\theta)T - m_1 - \ldots - m_{n-1})\big)$ has to be inserted in the sum (where $\nu(\theta)$ is the sum of the absolute values of the winding numbers of the circuits in θ).

The above considerations show that the contributions to $G_\Lambda(s)$ form a power series in the variable $z = kU^{-1}$. The terms of order $n-1$ come from the contributions of the truncated functions for the clusters θ with number of jumps $j(\theta) = n$. If the convergence condition for the cluster expansion is satisfied, which in the particular case $\mu_e - U = 0$, being considered, means that $U > 2d(1 + C_0)k$, then this series convergent. ¿From the convergence of $F_x(s)$ it follows that

(P0)
$$\sum_{A: x \in A} |\Phi_A(s_A)| < \infty$$

We have also, in particular, the following properties

(P1)
$$\sum_{n \geq 4} |\Phi^{(n)}_{\{x,y\}}(s_{\{x,y\}})| < k^4 U^{-3} B_1$$

(P2)
$$\sum_{A: \substack{x \in A \\ |A| \geq 3}} |\Phi_A(s_A)| < k^4 U^{-3} B_2$$

These inequalities are uniform, that is the constants B_1 and B_2 are independent of the site x and of the configuration s.

We assume the following hypothesis

(H1)
$$U > 2d(1 + C_0)k, \quad \mu_e - U = 0$$

(H2)
$$1 > 4k^2 U^{-2} B_0$$

Condition (H1) is the convergence condition of Theorem 1, in the particular case $\mu_e - U = 0$ which is being discussed. Condition (H2), where $B_0 \geq B_1 + B_2$, is assumed in order to use properties (P1) and (P2) above. Both conditions can be satisfied if U is sufficiently large.

Let us rewrite the effective interaction energy to make apparent the inverse temperature β. This means that k and U are replaced, respectively, by βk and βU. Then, up to a constant term,

$$\beta G_\Lambda(s) = -\frac{\beta}{2}(\mu_n - \mu_e) \sum_{x \in \Lambda} s(x) + \frac{\beta k^2}{4U} \sum_{|x-y|=1} s(x)s(y) + R_\Lambda(s)$$

The terms of order U^{-3} are included in $R_\Lambda(s)$.

Consider the case of a square lattice $\mathcal{L} = \mathbb{Z}^2$. The lattice may be broken up in two sublattices $\mathcal{L}_1$ and $\mathcal{L}_2$ with the property that all nearest neighbours of a site on sublattice $\mathcal{L}_1$ belong to the sublattice $\mathcal{L}_2$ and viceversa. For $R_\Lambda(s) = 0$ the hamiltonian above is that of the Ising antiferromagnet. In the region $(1/2)|\mu_n - \mu_e| < k^2U^{-1}$, there are two ground configurations: (1) $s(x) = 1$ if x is on the $\mathcal{L}_1$ sublattice and $s(x) = -1$ if x is on the $\mathcal{L}_2$ sublattice, and (2) $s(x) = -1$ if x is on the $\mathcal{L}_1$ sublattice and $s(x) = 1$ if x is on the $\mathcal{L}_2$ sublattice. The nuclei are placed like the black squares on a chess board.

The effect of the terms in $R_\Lambda(s)$ can be controlled by using the estimates discussed above. This leads to the proof of the following proposition for the Falicov-Kimball model. As we have already mentioned, the convergence condition of Theorem 1, instead of (H1), would be sufficient for obtaining this result.

Theorem 2. *Assume that conditions (H1) and (H2) are satisfied. Then, for μ_n and μ_e in the region*

$$(1/2)|\mu_n - \mu_e| < k^2U^{-1}(1 - 4k^2U^{-2}B_0)$$

the ground state configurations for the nuclei subsystem are the two chess board configurations just described. Moreover, under the same conditions and in the same region, we have that, given δ, with $0 < \delta < 1/2$, one can find a positive constant β_0, independent of the size of the box Λ, such that for any inverse temperature $\beta > \beta_0$, there are two Gibbs states ρ_1 and ρ_2, which satisfy $\rho_1(s(x)) \le -1 + \delta$ for $x \in \mathcal{L}_1$ and $\rho_1(s(x)) \ge 1 - \delta$ for $x \in \mathcal{L}_2$, the symmetric relations being satisfied by ρ_2.

This result says that in the infinite volume limit there will be two phases, in which the long range order of the chess board type continues to exist, if the temperature is low enough. We recover the result in Ref. 3, Theorem 1.

To prove these facts we use, as in Ref. 3, a Peierls type argument, adapted by Dobrushin [10] to treat the antiferromagnetic Ising model in the presence of an external field. On the boundary of the box Λ, let $s(x) = 1$ if $x \in \mathcal{L}_1$ and $s(x) = -1$ if $x \in \mathcal{L}_2$. In the interior contours are drawn between pairs of adjacent sites x and y if $s(x) = s(y)$.

The probability $\langle s(\gamma)\rangle$ of the occurrence of a contour of length $|\gamma|$ is estimated as follows. Let s be a configuration in which this contour γ occurs, and transform this configuration in the configuration $s^* = D_\gamma s$ defined as follows. If $x \in \Lambda$, let x' be the site just below it. For x outside γ, $s^*(x) = s(x)$, while if both x and x' are inside γ, $s^*(x) = s(x)$. However for x inside γ and x' outside, $s^*(x) = -s(x)$. The effect of this transformation, which leaves the configuration outside γ unchanged, is to eliminate the contour γ while shifting all contours lying inside γ by one step in the vertical direction. The energies are related by

$$G_\Lambda(s^*) \le G_\Lambda(s) - \frac{k^2}{2U}|\gamma| + \frac{1}{4}|\mu_n - \mu_e||\gamma| + \Delta$$

where the second term in the right hand side is the energy lost in eliminating the contour γ due to the nearest neighbour interaction, the third bounds the change in the energy due to the term involving $\frac{1}{2}(\mu_n - \mu_e)$, and Δ is the change in the energy due to all remaining potentials. For Δ we have the bound

$$\Delta \leq k^4 U^{-3} B_0 |\gamma|$$

Properties (P1) and (P2) are just what is needed to estimate the difference of energies between the configurations s and s^* due to the potentials included in R_Λ. Property (P1) bounds the corrections due to the higher order nearest neighbour interactions, and (P2) bounds the corrections due to the potentials of range strictly larger than one. Notice that only the interaction potentials Φ_A for which A contains a site at distance $1/2$ from the contour γ appear in the difference of energies. The exponential corrections containing the term $e^{-\beta U}$ (recall that U has been replaced by βU), which appear in $\Phi^{(2)}_{\{x,y\}}$ and $\tilde{\Phi}^{(2)}_{\{x,y\}}$, can be included (for large U or β) in the term $k^4 U^{-3} B_0$. The conclusion is that

$$\langle s(\gamma) \rangle \leq \exp\Big(- \beta \big(\frac{k^2}{2U} |\gamma| - \frac{1}{4} |\mu_n - \mu_e| |\gamma| - 2k^4 U^{-3} B_0 |\gamma| \big) \Big)$$

We can now apply the standard Peierls argument to derive the stated result, provided that β is large enough and that conditions (H1), (H2) and (H3) are satisfied. The value of β_0 can also be obtained from the above formulas. The Theorem is proved.

Of course similar arguments can be carried out for the three dimensional cubic lattice, or more generally, for other regular bipartite lattices which can be decomposed in a similar way into two sublattices.

Having studied the effective interaction energy to the first order in U^{-1}, we next examine the following terms of order U^{-3}. The study will be carried out for the cubic lattice $\mathcal{L} = \mathbb{Z}^d$ in dimension $d \geq 2$. These terms are obtained by taking into account the clusters with four jumps (see Fig. 2). We shall first consider only non-winding circuits.

Let $A = \{x, y\}$ be a set of two adjacent sites. If $s(x) = -s(y)$ a cluster θ, with $j(\theta) = 4$ and $\pi(\theta) = \{x, y\}$, can be constructed with two intersecting circuits ω_1 and ω_2 such that $j(\omega_1) = j(\omega_2) = 2$. Such clusters contribute to $\Phi^{(4)}_{\{x,y\}}$.

If $A = \{x, y, z\}$ is a set of three sites such that y is adjacent to x and to z, the clusters such that $j(\theta) = 4$ and $\pi(\theta) = \{x, y, z\}$, can be made either with only one circuit ω such that $j(\omega) = 4$, or with two intersecting circuits ω_1 and ω_2 such that $j(\omega_1) = j(\omega_2) = 2$ and $\pi(\omega_1) = \{x, y\}$, $\pi(\omega_2) = \{y, z\}$. Taking the orientations into account, one sees that the first case applies when $s(x) = s(y) = -s(z)$ or $-s(x) = s(y) = s(z)$, the second when $s(x) = -s(y) = s(z)$. Such clusters contribute to $\Phi^{(4)}_{\{x,y,z\}}$.

Finally, if $A = P = \{x, y, z, w\}$ is the set of the four sites on a unit square of the lattice, clusters such that $j(\theta) = 4$ and $\pi(\theta) = P$ exist, except in the case in which $s(x) = s(y) = s(z) = s(w)$. They consist of only one circuit ω with $j(\omega) = 4$. If $s(x)s(y)s(z)s(w) = 1$, we have, for such circuits, $\alpha(\omega) = -1$. Such clusters contribute to $\Phi^{(4)}_P$.

The components of the interaction potentials are given by

$$\Phi^{(4)}_A(s_A) = \lim_{T \to \infty} \sum_{\substack{\theta : \pi(\theta) = A \\ j(\theta) = 4}} \varphi^C_s(\theta)$$

The result of this computation is the following

$$
\begin{aligned}
G_\Lambda^{(3)}(s) = -\frac{1}{2}(\mu_n - \mu_e)\sum_x s(x) + \big(\frac{k^2}{4U} - \frac{9k^4}{16U^3}\big) \sum_{|x-y|=1} s(x)s(y) \\
+\frac{3k^4}{16U^3} \sum_{|x-y|=\sqrt{2}} s(x)s(y) + \frac{k^4}{8U^3} \sum_{|x-y|=2} s(x)s(y) \\
+ \frac{5k^4}{16U^3} \sum_P s(x)s(y)s(z)s(w)
\end{aligned}
$$

The summation in the last term goes over the unit squares of Λ. Then $G_\Lambda(s) = G_\Lambda^{(3)}(s) + R_\Lambda(s)$, where the rest R_Λ is of order U^{-5}.

This expression coincides with formula (3.46) of Ref. 5, where it was found, for the dimension $d = 2$, by means of the formal perturbation theory. The argument above proves it for any dimension $d \geq 2$. Let us mention that the computations which lead to this expression have also been done, with the method described here, and have been extended to other cases, by Merkli [11].

The ground state configurations associated to the approximate hamiltonian $G_\Lambda^{(3)}(s)$ have also been examined in Ref. 5 in the case of the square lattice $\mathcal{L} = \mathbb{Z}^2$. Besides the chess board configurations, $\mathcal{S}_{cb}$, for which the nuclei density is $\rho_n = 1/2$, three other kinds of periodic ground configurations, $\mathcal{S}_1$, $\mathcal{S}_2$, $\mathcal{S}_3$, with periods equal to 3, 4, 5, and having the densities $\rho_n = 2/3$, $3/4$ and $4/5$, are found, for $h = \frac{1}{2}(\mu_n - \mu_e) \geq 0$. For the opposite negative values of $h = \frac{1}{2}(\mu_n - \mu_e)$, the associated ground configurations (obtained by changing $s(x)$ into $-s(x)$) have densities $\rho_n = 1/3$, $1/4$ and $1/5$. These ground configurations are represented in Fig. 3 (taken from Ref. 5), the nuclei are placed on crystalline sublattices. They appear successively when $h = \frac{1}{2}(\mu_n - \mu_e)$ varies in intervals determined by four precise values

$$
\begin{aligned}
h_1 = k^2U^{-1} - \tfrac{21}{4}k^4U^{-3}, \quad h_2 = k^2U^{-1} - 3k^4U^{-3}, \\
h_3 = k^2U^{-1} - k^4U^{-3}, \qquad h_4 = k^2U^{-1} + \tfrac{1}{4}k^4U^{-3}.
\end{aligned}
$$

For $-h_1 < h < h_1$, the two chess board configurations, $\mathcal{S}_{cb}$, are the ground configurations. For $h_1 < h < h_2$, $h_2 < h < h_3$ and $h_3 < h < h_4$, respectively, the configurations of $\mathcal{S}_1$, $\mathcal{S}_2$ and $\mathcal{S}_3$, with densities $\rho_n = 2/3$, $3/4$ and $4/5$, are the only periodic ground configurations. All these intervals have length of order U^{-3}. For $h > h_4$, the only periodic ground configuration is $\mathcal{S}_+$, with $s(x) = 1$ for all $x \in \Lambda$, and density $\rho_n = 1$.

A proof of these facts will be given below, in Appendix 3. Actually, the ground state diagram has not been completely proved in Ref. 5. Proofs are given for h outside a certain interval (h_2', h_3'), where $h_2' < h_2$ and $h_3' > h_3$, while for h inside this interval the ground states, and in particular the states $\mathcal{S}_2$, are only conjectured.

As we have mentioned in the Introduction, Kennedy [6], in a recent study of the ground states of the Falicov-Kimball model at fixed densities. has rigorously justified the existence of these same ground configurations, when U is sufficiently large,

The following Theorem extends to the Falicov-Kimball model on the square lattice the analysis of the ground state diagram given in Appendix 3, Proposition 1. We notice that such a result can also be obtained by assuming, instead of condition (H1), the convergence condition of Theorem 1.

Theorem 3. *Assume that condition (H1) is satisfied, and let h be chosen in one of the following intervals*

$$h_\ell + \eta_\ell < h = \frac{1}{2}(\mu_n - \mu_e) < h_{\ell+1} - \eta_\ell$$

for $\ell = 0, 1, 2, 3, 4$, where the η_ℓ are some positive quantities of order U^{-5}. Here $h_0 = -h_1$ and $h_5 = +\infty$. Then, if U is sufficiently large (condition (H3), to be stated below), the periodic ground state configurations of the nuclei subsystem coincide with the ground configurations $\mathcal{S}_{cb}$, $\mathcal{S}_1$, $\mathcal{S}_2$, $\mathcal{S}_3$ and $\mathcal{S}_+$, described above, which are associated with the same value of h. For the opposite negative values of h, the associated periodic ground state configurations are obtained by changing $s(x)$ into $-s(x)$. Moreover, the Peierls condition is satisfied.

We shall prove the Theorem for h in the interval $h_1 < h < h_2$. This corresponds to the case of the ground configurations $\mathcal{S}_1$. The analogous results for the ground configurations $\mathcal{S}_{cb}$, $\mathcal{S}_2$, $\mathcal{S}_3$ and $\mathcal{S}_+$ follow by the same arguments.

It is shown, in the proof of Proposition 1, Appendix 3, that, for these values of h, the configurations denoted by $\bar{s}_2$, $\bar{s}_3$, $\bar{s}'_2$ and $\bar{s}'_4$, are the configurations (on the bonds P and B), for which a strict minimum of the interaction potentials is attained. We call them the good bond configurations. Any other configuration on P or B is wrong, in the sense that it increases the energy by a positive quantity. This quantity is larger than

$$D_0 k^4 U^{-3} \tau, \quad \text{with} \quad \tau = k^{-4} U^3 \min\{h - h_1, h_2 - h\}$$

where $D_0 > 0$ is a uniform constant. ¿From the definition, we have $0 < \tau < 9/8$.

Consider now on the finite lattice $\Lambda \subset \mathbb{Z}^2$ the subset of all squares of side $L = 3$ (to be called large squares). Given a configuration s in Λ, we classify the large squares into two classes $E_1(s)$ and $E_2(s)$. Either, the configuration s, restricted to the square, coincides with the restriction of one of the ground configurations, and then we say that the square belongs to $E_1(s)$, or, the configuration s, restricted to the square, does not coincide with any ground configuration, and then we say that the square belongs to $E_2(s)$. Connected sets of squares of the second class are considered as contours. In fact, if two adjacent large squares of class $E_1(s)$, correspond to two different ground configurations, then, all other large squares, that contain their common side, belong to $E_2(s)$.

All squares in $E_2(s)$ contain some wrong bond configuration (or part of it in the case of B-bonds) and, since any given bond is shared at most by 12 large squares, each square in $E_2(s)$ contributes to increase the energy by at least $(1/12)D_0 k^4 U^{-3} \tau$ (with respect to the ground state energy).

To continue the proof one has to take into account and to estimate the effect of the higher order terms appearing in R_Λ. This can be done, if the appropriate conditions are assumed, with the help of the cluster expansion properties. We have the following bound

$$\text{(P3)} \qquad \sum_{A,n:\, \substack{x\in A \\ n\geq 6}} |\Phi^n_A(s_A)| < B_3 k^6 U^{-5}$$

on the contributions of all clusters with number of jumps $n \geq 6$, where the constant $B_3 > 0$ is independent of s and x. We assume that B_3 is chosen such that the bound $B_3 k^6 U^{-5}$ accommodates also the contribution of winding clusters with $n \leq 4$ jumps and the other exponential corrections due to the finite size of the considered clusters.

These properties hold if condition (H1), the convergence condition (in the case $\mu_e - U = 0$ being considered), is satisfied. Then, given any configuration $s \in Q(\Lambda)$, the correction to $G^{(3)}_\Lambda(s)$, to get the exact effective energy $G_\Lambda(s)$, amounts at most to $B_3 k^6 U^{-5}$ per large square inside Λ (each large square contains 16 sites but each site is shared by 16 large squares). Besides condition (H1), we assume

$$\text{(H3)} \qquad (9/8)D_0 > 24\ B_3 k^2 U^{-2}$$

(by choosing U sufficiently large) and consider the region defined by

$$\Delta = D_0\tau - 24\ k^2 U^{-2} B_3 > 0$$

This region is non empty because of condition (H3) and corresponds to take h in an interval $h_1 + \eta_1 < h < h_2 - \eta_1$, with $\eta_1 > 0$ of order U^{-5}. It follows from the above discussion, that, for h in the region defined by $\Delta > 0$, each large square in $E_2(s)$ (which, therefore forms part of a contour) contributes to a positive increment of the energy, of at least $\Delta k^4 U^{-3}$, with respect to the ground state energy. This proves (for such values of h) that the Peierls condition is satisfied by the ground configurations $\mathcal{S}_1$. The Theorem is proved.

The ground states, in the intervals of h that have been analysed, are periodic and have nuclei densities $\rho_n = 0,\ 1/5,\ 1/4,\ 1/3,\ 1/2,\ 2/3,\ 3/4,\ 4/5,\ 1$. These domains are separated by small intervals with length of order U^{-5}. By considering higher order approximations in the nuclei effective interaction, new periodic ground states may be expected inside these small intervals. This led to conjecture, in Ref. 5, that the exact ground state phase diagram has a kind of devil's staircase structure, which divides the values of h into domains where the nuclei configurations are periodic, with increasing densities as h is increased.

We may expect that if the temperature is low enough (i. e., if $\beta > \beta_0$, where β_0 is some constant) then, several Gibbs states coexist, which could be analysed for h inside the intervals considered in Theorem 3. Each state being associated to one of the ground configurations, corresponding to the considered value of h, and having long range order properties near to those of the ground configuration. The analysis of the low temperature states, which can be regarded as a particular case in the Pirogov-Sinai theory, will not be discussed here. The possibility of extending this theory to the present case, which includes long range potentials, along the lines of Refs. 12, 13 and 14, appears very plausible using the strong decay properties of these potentials.

Let us finally remark that the possible applications of the cluster expansion method developed in the present work go beyond the particular cases that have been discussed in this Section. The fact that it permits to compute the effective interaction energy of the nuclei subsystem at different orders, having at the same time a full control on the corrections coming from the higher order terms, explains why this method can be useful to yield rigorous information on other problems concerning the Falicov-Kimball model or other related models.

4. Appendix 1

In this Appendix we study the path integral representation of the model. We shall, in fact, study a system more general than the Falicov-Kimball model, defined as follows. Let Λ be a finite box on the cubic lattice $\mathbb{Z}^d$. Consider on Λ two kinds of Fermi particles (indices 1 and 2). Let $\mathcal{F}(\Lambda)$ be the corresponding Fock space, and let $c_\sigma^+(x)$, $c_\sigma(x)$, $\sigma = 1, 2$ be the creation and annihilation operators of a particle at the point $x \in \Lambda$. We have the anticommutation relations $c_\sigma^+(x)c_\sigma(y) + c_\sigma(y)c_\sigma^+(x) = \delta_{x,y}$, $c_\sigma(x)c_\sigma(y) + c_\sigma(y)c_\sigma(x) = 0$ for $\sigma = 1, 2$ and operators with different particle indices commute. We consider the following hamiltonian

$$H = -k_1 \sum_{|x-y|=1} c_1^+(x)c_1(y) - k_2 \sum_{|x-y|=1} c_2^+(x)c_2(y) + 2U \sum_x n_1(x)n_2(x)$$

where k_1 and k_2 are the hopping coefficients (we assume that the two kinds of particles may have different masses), U gives the interaction when two particles are at the same point, and $n_\sigma(x) = c_\sigma^+(x)c_\sigma(x)$, $\sigma = 1, 2$, are the number operators. The Hubbard model corresponds to the case $k_1 = k_2$, $\sigma = 1, 2$ representing the two spin states of the electrons (in this case the creation and annihilation operators with different indices anticommute).

In the expression of H, the first two terms represent the kinetic energy H_0 and the last term is the potential energy. The decomposition

$$H = H_0 + V$$

will be used later. The total number operators

$$N_\sigma = \sum_x n_\sigma(x), \quad \sigma = 1, 2$$

commute with the hamiltonian and are constants of motion.

In the canonical ensemble the system is restricted to the subspaces $\mathcal{F}_{m,n}(\Lambda)$ of $\mathcal{F}(\Lambda)$ where the numbers of each kind of particles are fixed, or, to the subspace $\mathcal{F}_N(\Lambda)$ in which the total number of particles, $N = m + n$, is fixed. The integer N may vary from 0 to $2|\Lambda|$. The particular case in which $N = |\Lambda|$ plays an important role and corresponds the half filled band.

We are going to develop the Feynman-Kac or path integral representation of the model. For this purpose it will be convenient to introduce the set $\mathcal{C}(\Lambda)$ of classical configurations associated to the system. A classical configuration $X \in \mathcal{C}(\Lambda)$ is specified by a pair $X = (X_1, X_2)$, where $X_1 = (x_1, \ldots, x_m)$ and $X_2 = (x'_1, \ldots, x'_n)$ are two finite sequences of distinct points in Λ. If the sequences have lengths respectively equal to m and n we say that the configuration belongs to the subset $\mathcal{C}_{m,n}(\Lambda)$. We also introduce the vacuum vector $|\emptyset\rangle \in \mathcal{F}(\Lambda)$ and the vector states $|X\rangle \in \mathcal{F}(\Lambda)$, associated to $X \in \mathcal{C}(\Lambda)$, as follows

$$|X\rangle = c_1^+(x_1) \ldots c_1^+(x_m) c_2^+(x'_1) \ldots c_2^+(x'_n)|\emptyset\rangle$$

We remark that

$$V|X\rangle = v(X)|X\rangle$$

where $v(X)$ is $2U$ times the number of common points in the sequences X_1 and X_2.

We introduce the notion of trajectories. Let t be an integer variable, $0 \leq t \leq T$, which will be called the time. A trajectory $x = x(t)$ is a sequence $x(0), x(1), \ldots, x(T)$ of sites in Λ, such that, for all $t = 0, 1, ..., T-1$, either $x(t+1) = x(t)$ or $x(t+1)$ is a neighbour of $x(t)$. This last case we describe as a jump. A configuration of trajectories is a sequence

$$X(t) = (X_1(t), X_2(t)) = (x_1(t), ..., x_m(t); x'_1(t), ..., x'_n(t))$$

of classical configurations, such that, for all $i = 1, ..., m$ and $j = 1, ..., n$, the sequences $x_i(t)$ and $x'_j(t)$, indexed by t, are trajectories.

Let $\mathcal{T}(\Lambda)$ be the set of configurations of trajectories, or a subset of the set of such configurations with specified number of particles. For a configuration of trajectories Δ, let $j_1(\Delta)$ and $j_2(\Delta)$ be the total number of jumps in the trajectories of X_1 and X_2, , respectively.

Then, from Troter's formula, which applied to the operator $\exp(-H)$, asserts

$$\exp[-(H_0 + V)] = \lim_{T\to\infty} \left(\exp(-\frac{V}{T})(1 - \frac{H_0}{T}) \right)^T$$

we get

$$\exp(-H)|X\rangle = \sum_{\Delta \in \mathcal{T}(\Lambda), X(0)=X} \exp\left(-\sum_{t=1}^{T} \frac{v(X(t))}{T} \right) \left(\frac{k_1}{T} \right)^{j_1(\Delta)} \left(\frac{k_2}{T} \right)^{j_2(\Delta)} |X(T)\rangle$$

In order to simplify the notations we include the inverse temperature factor β in the coupling constants of the hamiltonian H

The set $\mathcal{T}(\Lambda)$ may be interpreted as the set of configurations of the quantum system. These configurations build a subset of classical configurations in a box $\Omega = \Lambda \times [0, T]$ on a $(d+1)$-dimensional lattice.

If in the above expression one replaces the vector $|X(T)\rangle$ by the scalar product $\langle X(0)|X(T)\rangle$, then one sums these expressions over all configurations $\Delta \in \mathcal{T}(\Lambda)$, and divides by the appropriate factorials, one obtains the partition function

$$Z(\Lambda) = \mathrm{Tr}\exp(-H)$$

Because $\langle X(0)|X(T)\rangle \neq 0$ only if $\mathrm{supp}X_\sigma(0) = \mathrm{supp}X_\sigma(T)$ for $\sigma = 1, 2$ (the support of a sequence is the set of its sites), all trajectories that contribute to the partition function are closed lines on the cylinder Ω^{per}, obtained from Ω by identifying the points $(x, 0)$ and (x, T) for all $x \in \Lambda$. ¿From the definition of the states $|X\rangle$ and the anticommutation relations, it follows that $\langle X(0)|X(T)\rangle = (-1)^{\pi_1+\pi_2}$, where $(-1)^{\pi_\sigma}$, for $\sigma = 1, 2$, is the parity of the permutation $X_\sigma(0) \to X_\sigma(T)$.

The reduced density matrices, describing the equilibrium states, can also be expressed as classical expectation values by means of the configurations of trajectories considered above.

Let us now discuss a geometric representation of these facts [a]. A trajectory $x(0), x(1), \ldots, x(T)$ corresponds to a continuous line on Ω^{per}, starting at the point $(x(0), 0)$ and ending at the point $(x(T), T)$. It consists of the vertical bonds $[(x(t), t), (x(t), t+1)]$, for $t = 0, ..., T-1$, and the horizontal bonds $[(x(t-1), t),\ (x(t), t)]$ if $x(t-1) \neq x(t)$, i.e., when there is a jump. A configuration $\Delta \in \mathcal{T}(\Lambda)$ is represented as the set of the corresponding trajectories. We distinguish the two kinds of particles by placing up-arrows on the trajectories of $X_1(t)$ and down-arrows on the trajectories of $X_2(t)$. For a later use, also the horizontal segments of a trajectory get an arrow, which follows the orientation of the trajectory. Each bond never belongs to more than one trajectory of each kind, but can belong to two trajectories with opposite arrows.

For each $t = 0, 1, ..., T-1$, one of the following cases occurs:

(1) If $x \in \mathrm{supp}X_1(t)\backslash\mathrm{supp}X_2(t)$, a trajectory with up-arrows goes along the vertical bond $b = [(x, t),\ (x, t+1)]$. We may say that x is occupied by a particle with index $\sigma = 1$ at time t.

(2) If $x \in \mathrm{supp}X_2(t)\backslash\mathrm{supp}X_1(t)$, a trajectory with down-arrows goes along b, and x is occupied by a particle with index $\sigma = 2$.

(3) If $x \in \mathrm{supp}X_1(t) \cap \mathrm{supp}X_2(t)$, two trajectories with opposite orientations intersect along b, and x is occupied by two different particles.

(4) If $x \in \Lambda\backslash(\mathrm{supp}X_1(t) \cup \mathrm{supp}X_2(t))$, there is no trajectory on b, and x is empty.

We may represent these situations as follows (see Fig. 4). In case (1) we draw on the vertical bond $b \in \Omega^{\mathrm{per}}$ a continuous segment with an up-arrow, in case (2) we draw a continuous segment with a down-arrow, in case (3) we draw a dashed segment with an up-arrow, and in case (4) we draw a dashed segment with a down-arrow. We complete the representation with some additional horizontal segments. On the horizontal bonds at which a jump takes place we draw a continuous segment, with the same arrow as the trajectory going along this bond, and a dashed segment, with an arrow in the direction of the jump.

[a] This representation was introduced by A. Messager, S. A. Pirogov and Y. Suhov

We denote by $\{\omega_1, ..., \omega_r\}$, the set of maximally connected components of dashed segments, and by $\{\omega'_1, ..., \omega'_s\}$, the set of maximally connected components of continuous segments. It is not difficult to see that all the components ω and ω' are closed self-avoiding paths, and that in each of them all arrows follow a common direction. We shall call these objects oriented circuits.

Notice that all vertical bonds on $\Omega^{\rm per}$ have a segment of some circuit and that two circuits of different kind (dashed and continuous) always meet along the horizontal segments of the circuits. Some of the circuits may close by winding around the cylinder $\Omega^{\rm per}$. On the other hand there is a one-to-one correspondence between the quantum configurations and such families of circuits. Moreover, any orientation can be given to any circuit since this leads to a new admissible configuration.

We also remark that the symmetries of the model are easy to see in this circuit representation. For instance, the change of sign of the constant U, which physically means to change the on-site repulsion between particles of different kind, into an attraction, is geometrically equivalent to interchange the role between the continuous and the dashed circuits.

A circuit ω is determined by the set of its vertices

$$\xi_0 = (x_0, t_0), \xi_1 = (x_1, t_1), ..., \xi_l = (x_l, t_l)$$

where l is an even number and $\xi_0 = \xi_l$. Alternatively, we have $t_i \neq t_{i+1}$ with $x_i = x_{i+1}$, and $t_j = t_{j+1}$ together with the fact that x_j and x_{j+1} are neibouring points. The number of jumps is equal to the number of horizontal segments and, we define the length of a circuit $|\omega|$, as the number of its vertical segments. If ω is a dashed circuit we denote by $J_1(\omega)$ the set of its horizontal segments whose orientation coincides with the orientation of the continuous segment which lies on the same bond, and by $J_2(\omega)$ the set of its horizontal segments for which the corresponding orientations are opposed. We denote by $j_1(\omega)$ and $j_2(\omega)$ the number of elements in $J_1(\omega)$ and in $J_2(\omega)$, respectively.

Assume, now, that the half filled band condition holds. That is, consider the canonical formalism with fixed total number of particles $N = |\Lambda|$. In this case, for any quantum configuration and at any $t \in [0, T]$, the total numbers of vertical dashed segments with down arrows and with up arrows, coincide. Recall that the term $v(X(t))$ is equal to the total number of vertical dashed segments with up arrows, that the configuration have between t and $t+1$, multiplied by $2U$. Then, the contribution of a given circuit configuration to the operator $\exp(-H)$ is

$$\prod_{\omega} \exp(-\frac{U}{T}|\omega|) \left(\frac{k_1}{T}\right)^{j_1(\omega)} \left(\frac{k_2}{T}\right)^{j_2(\omega)} \prod_{\omega}{}' A(\omega)$$

where the product is over all oriented dashed circuits of this configuration, and

$$\prod_{\omega}{}' A(\omega) = \mathcal{T} \prod_{\omega} \prod_{(\xi_i,\xi_{i+1}) \in J_1(\omega)} c_1^{+}(x_{i+1}) c_1(x_i) \prod_{(\xi_i,\xi_{i+1}) \in J_2(\omega)} c_2^{+}(x_{i+1}) c_2(x_i)$$

The symbol $\mathcal{T}$ means that the product is chronologically ordered. That is, it is assumed that the time variable implicit in the ξ indicates that, in product giving $\exp(-H)$, the operator factors, coming from the $A(\omega)$, have to be ordered from right to left according to the sequence of increasing times.

It can be observed that the weight of the dashed circuits decreases exponentially with U (this is better seen once the limit $T \to \infty$ has been performed) and with their length. This means that, under the half filled condition, the dashed circuits have small probability for large U. On the other side, if we specify the configuration of the dashed circuits, then, the configuration of the continuous circuits, which can be associated to this configuration of dashed circuits, is geometrically determined, only the orientation of each continuous circuit has to be given. This means that we have 2^M possible configurations, where M is the number of different continuous circuits (without orientations) that appear in the configuration. However, this number M (i. e., the number of maximally connected components in the set of continuous unit segments) is a rather complicated function of the configuration of dashed circuits. Another difficulty comes from the sign of the Boltzmann factor associated to this configuration.

In the particular case in which the hopping coefficient k_1 equals 0, which corresponds to the Falicov-Kimball model, the situation is much more simple. In this case all the horizontal segments of a dashed circuit belong to the set $J_2(\omega)$, and the set $J_1(\omega)$ is empty. A configuration of dashed circuits is possible (i. e., gives a non zero contribution) if, and only if, for each vertical line (x,t) in the box $\Omega^{\rm per}$, where $x \in \Lambda$ is a fixed site and $t \in [0,T]$, all dashed circuits which intersect this line have the same orientation along it. Then, there exists a unique configuration for the oriented continuous circuits.

According to this fact, let us first give the orientation of the vertical lines. This can be done by choosing a classical spin configuration s on Λ, which to each site $x \in \Lambda$ assigns the values $s(x) = 1$ or $s(x) = -1$ according to whether the arrows on the vertical line (x,t), $t \in [0,T]$, go up or go down. We denote by $Q(\Lambda) = \{-1,1\}^\Lambda$ the set of such classical configurations. ¿From the discussion above we obtain

$$Z(\Lambda) = \lim_{T\to\infty} \sum_{s\in Q(\Lambda)} \sum_{\{\omega_1,\ldots,\omega_r\}} \prod_{q=1}^{r} \exp(-\frac{U}{T}|\omega_q|) \left(\frac{k_2}{T}\right)^{j_2(\omega_q)} \alpha(\omega_q)$$

where the second sum runs over all compatible families of oriented dashed circuits, $\{\omega_1,...,\omega_r\}$, which, moreover, are compatible with the configuration $s \in Q(\Lambda)$. The factor $\alpha(\omega_q)$ associated to each oriented dashed circuit is $+1$ or -1. It has the value of $\langle X_1(0)|X_1(T)\rangle$, where $X_1(0)$ and $X_1(T)$ are the initial and final classical configurations in $\mathcal{C}(\Lambda)$, associated with the quantum configuration in $\mathcal{T}(\Lambda)$ which contains only the oriented dashed circuit ω_q. The proof that the sign of each term, in the sum which defines the partition function, is the product of the signs $\alpha(\omega_q)$, attached to each circuit follows in a natural way from the definitions. These observations, for the case $k_1 = 0$, led us to the analysis developed in Section 2.

5. Appendix 2

In this Appendix we give a more detailed description of the cluster expansion considered in Section 2. We follow, as mentioned, the formalism of Ref. 8. For simplicity in the exposition we take $\mu_e = U$.

We introduce a new (positive) activity

$$\mu(\omega) = e^{-\frac{W}{T}|\omega|}\left(\frac{\lambda}{T}\right)^{j(\omega)}$$

for the (oriented dashed) circuits compatible with the configuration $s \in Q(\Lambda)$. Since we are computing $\tilde{Z}(\Lambda, s)$ only the circuits compatible with the given configuration s are considered. We write also $\varphi_s(\omega) = \varphi(\omega)$.

Let ω_0 be a given circuit. First, we are going to estimate the following sum

$$q(\omega_0) = \sum_S{}^{*} \mu(S) = \sum_S{}^{*} \prod_{\omega \in S} \mu(\omega)$$

extended to all sets S of circuits without intersections, such that all circuits in S intersect ω_0. Let $v_1, \ldots, v_{j_0}$, be the vertical lines of the circuit ω_0 and $m_1^{(0)}, \ldots, m_{j_0}^{(0)}$ their lengths ($j_0 = j(\omega_0)$ coincides with the number of jumps in ω_0).

There are vertical lines in ω_0, such as, say v_1, intersected by a circuit ω which covers all the line v_1. In this case, let $m_1, m_2, \ldots, m_l$, where $m_1 = m_1' + m_1^{(0)} + m_1''$, be the lengths of the vertical lines in ω. Then, we have

$$\begin{aligned}\sum_{v_1 \subset \omega}{}^{*} \mu(\omega) &\leq \sum_{l \geq 2} \sum_{m_1', m_1'', m_2, \ldots, m_{l-1}} e^{-\frac{W}{T}(m_1' + m_1'' + m_2 + \ldots + m_{l-1})}\left(\frac{\lambda}{T}\right)^l \\ &\leq \sum_{l \geq 2}\left(1 - e^{-\frac{W}{T}}\right)^{-l}\left(\frac{2d\lambda}{T}\right)^l \leq \left(\frac{2d\lambda}{W}\right)^2\left(1 - \left(\frac{2d\lambda}{W}\right)^2\right)^{-1} \leq C_1^2\end{aligned}$$

provided that $W \geq C^{-1} 2d\lambda$, with $C < 1$. Then $C_1^2 = C^2(1 - C^2)^{-1}$.

There are vertical lines in ω_0, such as say v_2, which are intersected by $0, 1, 2, \ldots$, etc., circuits. For each one of these circuits, say ω, there is a jump at one point of v_2. Observe that for the sum over the circuits with a jump at a given point ξ, we have

$$\begin{aligned}\sum_{\xi \in J(\omega)} \mu(\omega) &\leq 2 \sum_{l \geq 2} \sum_{m_1, m_2, \ldots, m_{l-1}} e^{-\frac{W}{T}(m_1 + m_2 + \ldots + m_{l-1})}\left(\frac{\lambda}{T}\right)^l \\ &\leq 2 \sum_{l \geq 2}\left(1 - e^{-\frac{W}{T}}\right)^{-(l-1)}\left(\frac{2d\lambda}{T}\right)^l \leq \frac{W}{T} 2C_1^2\end{aligned}$$

under the same condition on W. If there are ν_2 circuits intersecting the line v_2, one can choose the jump points in $\binom{m_2^{(0)}}{\nu_2}$ ways. Thus, in this case, for the circuits intersecting the line v_2, we get

$$\begin{aligned}\sum_S{}^{*} \mu(S) &\leq \sum_{\nu_2}^{\infty} \sum_{\omega_1, \ldots, \omega_{\nu_2}}{}^{*} \mu(\omega_1) \ldots \mu(\omega_{\nu_2}) \\ &\leq \sum_{\nu_2}^{\infty} \binom{m_2^{(0)}}{\nu_2}\left(\frac{2C_1^2 W}{T}\right)^{\nu_2} \leq e^{\frac{m_2^{(0)}}{T} 2C_1^2 W}\end{aligned}$$

Among the j_0 vertical lines of the circuit ω_0, there can be $j_1 = 0, 1, \ldots, j_0$, lines in which the first case occurs, and $j_2 = j_0 - j_1$ lines in which the second case occurs. The number of choices is $\binom{j_0}{j_1}$. Therefore

$$q(\omega_0) \leq \sum_{j_1=0}^{j_0} \binom{j_0}{j_1} C_1^{2j_1} e^{\frac{|\omega_0|}{T} 2C_1^2 W} \leq (1 + C_1^2)^{j(\omega_0)} e^{\frac{2C_1^2 W}{T} |\omega_0|}$$

Having established this property the discussion which follows is an easy adaptation of the method of Ref. 8 (Section 4). One defines, associated to the Boltzmann factor $\varphi(X)$, the function

$$\Delta_X(Y) = (\varphi^{-1} \dot{D}_X \varphi)(Y)$$

Here X, Y, are multiplicity functions on the set of circuits, the product is understood in the sense of the algebraic formalism described in Ref. 8, φ^{-1} is the inverse of φ in the sense of this product, and D_X is the derivation considered also in Ref. 8. The circuits of X have no intersections (otherwise $\Delta_X(Y) = 0$). We write $N(X) = \sum_\omega X(\omega)$ and $X! = \prod_\omega X(\omega)!$.

Let $\omega_0 + X$ be the multiplicity function corresponding to a set of circuits without intersections ($\omega_0(\omega') = 1$ if $\omega' = \omega_0$ and 0 otherwise). We can write the following equation, for Y arbitrary and X without overlapings,

$$\Delta_{\omega_0+X}(Y) = \varphi(\omega_0) \sum_{S \leq Y}{}^{*} (-1)^{N(S)} \Delta_{S+X}(Y - S)$$

This equation comes from the Minlos-Sinai equations, the integral or Mayer equations for polymers. The sum $\sum^*$ extends over all subsets S of Y such that all circuits in S intersect ω_0 and $X + S$ is a compatible set. The set $S = \emptyset$ has to be included in the sum and $\Delta_\emptyset(Y) = 1$. Let I_m be defined by

$$I_m = \sup_{\substack{\omega_1, \ldots, \omega_n \\ m \geq n \geq 1}} \sum_{\substack{Y \\ N(Y) = m-n}} |\Delta_{\omega_1, \ldots, \omega_n}(Y)| \mu^{-1}(\omega_1) \ldots \mu^{-1}(\omega_n)$$

Then, using the integral equation and the bound on $q(\omega_0)$, one obtains

$$\begin{aligned}
&\sum_{\substack{Y \\ N(X)+N(Y)=m}} |\Delta_{\omega_0+X}(Y)| \mu^{-1}(\omega_0) \mu^{-1}(X) \\
&\leq |\varphi(\omega_0)| \mu^{-1}(\omega_0) \sum_{S \leq Y}{}^{*} |\Delta_{X+S}(Y - S)| \mu^{-1}(X) \leq I_m \ |\varphi(\omega_0)| \mu^{-1}(\omega_0) \sum_{S}{}^{*} \mu(S) \\
&\leq I_m e^{-\frac{1}{T}(U - W - 2C_1^2 W)|\omega_0|} \left(\frac{k(1 + C_1^2)}{\lambda} \right)^{j(\omega_0)} \leq I_m r^m
\end{aligned}$$

where $r < 1$ provided that $\lambda = r^{\frac{1}{2}}(1 + C_1^2)k$ and $U \geq W(1 + 2C_1^2)$. Since it was assumed above that $W \geq C^{-1} 2d\lambda$ (with $C < 1$), this condition becomes

$$U > 2dC^{-1}(1 + 2C_1^2)(1 + C_1^2) r^{-\frac{1}{2}} k = 2d(1 + C_0)k$$

That is, the condition of Theorem 1 (for $\mu_e = U$). If this condition is satisfied, we thus conclude

$$I_{m+1} \leq I_m r, \quad \text{for } m \geq 1$$

and, because $I_1 = \sup_\omega |\varphi(\omega)|\mu^{-1}(\omega) \leq r$, we see that

$$I_m \leq r^m$$

This bound allows us to estimate the truncated functions φ^C as follows. ¿From $\Delta_\omega(X) = \varphi^C(\omega + X)((\omega + X)!/X!)$, we derive the following useful estimate

$$\sum_X |\varphi^C(\omega + X)| \leq \sum_{m=1}^{\infty} \sum_{N(X)=m-1} |\Delta_\omega(X)| \leq \sum_{m=1}^{\infty} I_m \mu(\omega) \leq r(1-r)^{-1}\mu(\omega)$$

¿From this, and taking into account the computations made at the begining of the Appendix, we can bound the sum over the clusters X, which contain a given point $\xi \in \Omega^{\text{per}}$, by

$$\sum_{\xi \in X} |\varphi^C(X)| \leq r(1-r)^{-1} \sum_{\xi \in \omega} \mu(\omega) \leq r(1-r)^{-1} C_1^2 = C_3$$

and the sum over the clusters X, whose projections $\pi(X)$ contain a given site $x \in \Lambda$, by

$$\sum_{x \in \pi(X)} |\varphi^C(X)| \leq r(1-r)^{-1} \frac{T}{2} \sum_{\xi \in J(\omega)} \mu(\omega) \leq r(1-r)^{-1} C_1^2 W = 2dC_4 k$$

Here $\xi \in \Omega^{\text{per}}$ and $\pi(\xi) = x$. The constant C_4 can be written in terms of the previous constants using that $W = 2dC^{-1}\lambda$ and $\lambda = r^{-\frac{1}{2}}(1 + C_1^2)k$.

This last estimate implies the following bound on the effective interaction for the nuclei subsystem

$$\sum_{x \in A} |\Phi_A(s_A)| \leq 2dC_4 k$$

and shows that it is a uniform bound, i. e., independent of the site $x \in \Lambda$ and of the configuration $s \in Q(\Lambda)$.

Applying the above results to the system defined by the circuit activities $\varphi'(\omega) = \varphi(\omega) R^{j(\omega)}$, one obtains also, for any $R > 0$,

$$\sum_{\xi \in X} |\varphi^C(X)| R^{j(X)} \leq C_3 \quad \text{and} \quad \sum_{x \in \pi(X)} |\varphi^C(X)| R^{j(X)-1} \leq 2dC_4 k,$$

if the condition $U > 2d(1 + C_0)Rk$ is satisfied.

6. Appendix 3

In this Appendix we study the ground states of the approximate hamiltonian $G_\Lambda^{(3)}$, giving the effective energy at the order U^{-3}. Besides the two chess board configurations $\mathcal{S}_{cb}$, and the configuration $\mathcal{S}_+$, with $s(x) = 1$ (for all $x \in \Lambda$), three other kinds of periodic configurations, $\mathcal{S}_1$, $\mathcal{S}_2$ and $\mathcal{S}_3$, with densities $\rho_n = 2/3$, $3/4$ and $4/5$, were introduced in Ref. 5, for the dimension $d = 2$. They are represented in Fig. 3 and can be described as follows. For the configurations $\mathcal{S}_1$, the sites where $s(x) = -1$ occupy the vertices of a crystalline sublattice generated by the vectors $e_1^{(1)} = (1,1)$ and $e_2^{(1)} = (2,-1)$. The choice of the origin and of the axes gives six different configurations in $\mathcal{S}_1$. For $\mathcal{S}_2$ and $\mathcal{S}_3$, the corresponding sublattices are generated by the vectors $e_1^{(2)} = (2,1)$, $e_2^{(2)} = (2,-1)$ and $e_1^{(3)} = (2,1)$, $e_2^{(3)} = (3,-1)$, respectively. We have the following Proposition.

Proposition 1. *Consider the hamiltonian $G_\Lambda^{(3)}$ on the square lattice $\mathcal{L} = \mathbb{Z}^2$, with U sufficiently large, and let $h = \frac{1}{2}(\mu_n - \mu_e)$. For*

$$-h_1 < h < h_1 = k^2U^{-1} - \tfrac{21}{4}k^4U^{-3},$$

the two chess board configurations, $\mathcal{S}_{cb}$, are the only periodic ground configurations. For

$$\begin{aligned} h_1 < h < h_2 &= k^2U^{-1} - 3k^4U^{-3}, \\ h_2 < h < h_3 &= k^2U^{-1} - k^4U^{-3}, \\ h_3 < h < h_4 &= k^2U^{-1} + \tfrac{1}{4}k^4U^{-3}, \end{aligned}$$

respectively, the configurations of $\mathcal{S}_1$, $\mathcal{S}_2$ and $\mathcal{S}_3$, with densities $\rho_n = 2/3$, $3/4$ and $4/5$, are the only periodic ground configurations. For $h > h_4$, the only periodic ground configuration is $\mathcal{S}_+$, with $s(x) = 1$ for all $x \in \Lambda$, and density $\rho_n = 1$. For the opposite negative values of h, the associated periodic ground state configurations (obtained by changing $s(x)$ into $-s(x)$) have densities $\rho_n = 1/3$, $1/4$, $1/5$ and 0. For $h = h_\ell$, with $\ell = 1,2,3,4$ (the values which separate the above intervals), the number of ground configurations is infinite.

We write

$$G_\Lambda^{(3)}(s) = \sum_P \frac{1}{16U^3}\Psi_P(s_P) + \sum_B \frac{1}{8U^3}\Psi_B(s_B)$$

as a sum of a four body potential Ψ_P, where the $P = \{x,y,z,w\}$ are, as before, the sets of the four sites of a unit square, and a five body potential Ψ_B, where $B = \{x_0,x,y,z,w\}$ are the sets, associated to a lattice site x_0 and build up with x_0 and its four adjacent sites. We introduce the variable

$$\delta = U^3(h - U^{-1})$$

and define these potentials by

$$\Psi_P(s_P) = \big(-\frac{9}{2} + \frac{a}{2}\big) \sum_{|x-y|=1} s(x)s(y) + (3+b) \sum_{|x-y|=\sqrt{2}} s(x)s(y)$$
$$+ 5\ s(x)s(y)s(z)s(w) + \frac{c}{4}\sum_x s(x)$$

$$\Psi_B(s_B) = -\frac{a}{4} \sum_{|x-y|=1} s(x)s(y) - \frac{b}{4} \sum_{|x-y|=\sqrt{2}} s(x)s(y)$$
$$+ \sum_{|x-y|=2} s(x)s(y) - \big(\frac{16\delta}{12} + \frac{c}{12}\big)\big(\sum_{x\neq x_0} s(x) + 2s(x_0)\big)$$

In order to simplify the notations we take $k = 1$. We shall consider, on the bonds P, the following configurations

$$\bar{s}_1 = \begin{matrix} \circ & \circ \\ \circ & \circ \end{matrix} \qquad \bar{s}_2 = \begin{matrix} \bullet & \circ \\ \circ & \circ \end{matrix} \qquad \bar{s}_3 = \begin{matrix} \bullet & \circ \\ \circ & \bullet \end{matrix}$$

and, on the bonds B,

$$\bar{s}'_1 = \begin{matrix} & \circ & \\ \circ & \circ & \circ \\ & \circ & \end{matrix} \qquad \bar{s}'_2 = \begin{matrix} & \circ & \\ \circ & \bullet & \circ \\ & \circ & \end{matrix} \qquad \bar{s}'_3 = \begin{matrix} & \bullet & \\ \bullet & \circ & \bullet \\ & \bullet & \end{matrix}$$

$$\bar{s}'_4 = \begin{matrix} & \bullet & \\ \bullet & \circ & \circ \\ & \circ & \end{matrix} \qquad \bar{s}'_5 = \begin{matrix} & \circ & \\ \bullet & \circ & \bullet \\ & \circ & \end{matrix} \qquad \bar{s}'_6 = \begin{matrix} & \circ & \\ \bullet & \circ & \circ \\ & \circ & \end{matrix}$$

where $\bullet = -1$ and $\circ = 1$. These configurations, and those which are related to them by a symmetry of the lattice, are characterized by the condition that on each pair of adjacent sites the configuration ($\bullet \quad \bullet$) is forbiden. Since the later configurations would increase the energy by terms of order U^{-1}, they do not appear in the ground states for U sufficiently large.

It will be shown that, according to the values of h being considered, some of these configurations (and those related to them by symmetry), are the configurations, on P and B, for which a strict minimum of the interaction potentials Ψ_P and Ψ_B is attained. We call them the good bond configurations associated to the considered value of h. Any other configuration on P or B (to be called a wrong bond configuration) increases the energy by a positive quantity. This implies that the ground state is made only with good bond configurations, and determines the structure of the periodic ground configurations.

We write

$$e_\ell = \Psi_P(\bar{s}_\ell), \quad \epsilon_\ell = \Psi_B(\bar{s}'_\ell)$$

Then, we have

$$e_1 = -7 + 2a + 2b + c, \quad e_2 = -5 + \tfrac{1}{2}c, \quad e_3 = 29 - 2a + 2b,$$

and, for $u = 16\delta + c$, we have, also,

$$\epsilon_1 = 2 - a - b - \tfrac{1}{2}u, \quad \epsilon_2 = 2 + a - b - \tfrac{1}{6}u, \quad \epsilon_3 = 2 + a - b + \tfrac{1}{6}u,$$

$$\epsilon_4 = -2 - \tfrac{1}{6}u, \qquad \epsilon_5 = 2 + b - \tfrac{1}{6}u, \qquad \epsilon_6 = -\tfrac{1}{2}a - \tfrac{1}{3}u.$$

Take $a = -8 + r$ and $b = -4 + r$. Then,

$$e_1 = -31 + 4r + c, \quad e_2 = -5 + \tfrac{1}{2}c, \qquad e_3 = 37,$$

$$\epsilon_1 = 14 - 2r - \tfrac{1}{2}u, \quad \epsilon_2 = -2 - \tfrac{1}{6}u, \qquad \epsilon_3 = -2 + \tfrac{1}{6}u,$$

$$\epsilon_4 = -2 - \tfrac{1}{6}u, \qquad \epsilon_5 = -2 + r - \tfrac{1}{6}u, \quad \epsilon_6 = 4 - \tfrac{1}{2}r - \tfrac{1}{3}u.$$

Take $c = 84$ and $r = 0$, and consider $u < 0$. Then, $e_2 = e_3 = 37 < e_1 = 53$ and $\epsilon_3 < \min_{\ell \neq 3} \epsilon_\ell$. Since $u = 16\delta + 84 < 0$ we see that, for $\delta < -\frac{21}{4}$, $\mathcal{S}_{cb}$ are the only ground state configurations.

Take $c = 84$ and $r > 0$ small. Consider $u > 0$ or, equivalently, $\delta > -\frac{21}{4}$. Then, again, $e_2 = e_3 < e_1$ and, also, $\epsilon_2 = \epsilon_4 < \min\{\epsilon_3, \epsilon_5\}$. If $u < 36 - 3r$, or, equivalently (since $c = 84$), if $\delta < -3 - \frac{3}{16}r$, we have $\epsilon_2 = \epsilon_4 < \epsilon_6 < \epsilon_1$. But one requires only that $r > 0$. Thus, for $-\frac{21}{4} < \delta < -3$, $\mathcal{S}_1$ are the only ground state configurations.

Let us choose now $u = 36$ and $r = 0$. With these values, we have

$$e_1 = -31 + c, \quad e_2 = -5 + \tfrac{1}{2}c, \quad e_3 = 37$$

$$\epsilon_1 = -4, \quad \epsilon_3 = 4, \quad \epsilon_2 = \epsilon_4 = \epsilon_5 = \epsilon_6 = -8.$$

Since $16\delta + c = u = 36$, we have that $e_2 < e_3$, if $\delta > -3$, and that $e_2 < e_1$, if $\delta < -1$. Thus, for $-3 < \delta < -1$, $\mathcal{S}_2$ are the only ground state configurations.

Finally, let $c = 52$ (and $r = 0$). Then, $e_1 = e_2 = 21 < e_3 = 37$. On the other hand, we have $\epsilon_6 < \epsilon_2 = \epsilon_4 = \epsilon_5 < \epsilon_3$, provided that $4 - \frac{1}{3}u < -2 - \frac{1}{6}u$. That is, for $u > 36$, or, equivalently (since $c = 52$), for $\delta > -1$. Furthermore, $\epsilon_2 < \epsilon_1$ for $u < 48$, that is, for $\delta < -\frac{1}{4}$. Therefore, for $-1 < \delta < -\frac{1}{4}$, $\mathcal{S}_3$ are the only ground state configurations. Next, we rely on the results of Ref. 5, where it has been proved that for $-\frac{5}{8} < \delta < \frac{1}{4}$, $\mathcal{S}_3$ are the only ground state configurations, and that for $\delta > \frac{1}{4}$, $\mathcal{S}_+$ is the only ground state configuration. The later statement determines the region associated to $\mathcal{S}_+$, the former, together with the previous result, allows us to assert that for $-1 < \delta < \frac{1}{4}$, $\mathcal{S}_3$ are the only ground state configurations. The last statement in the Proposition follows from the fact that, at the values $h = h_\ell$, there is a larger number of good bond configurations. The Proposition is proved.

The properties of the effective interaction used in the above proof show that the hamiltonian $G_\Lambda^{(3)}(s)$, can be written as an m-potential. These properties are needed, also, in Section 3, in the proof of the Peierls condition (Theorem 3). The above proof is a continuation of the analysis in Ref. 5, Section 3.3. Possibly similar arguments could be applied to the case of the cubic lattice $\mathcal{L} = \mathbb{Z}^3$ extending to this case the study of the ground states of the model.

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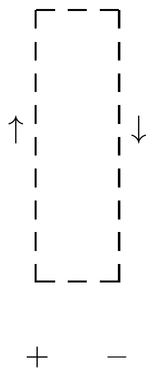


Fig. 1. The simplest circuit

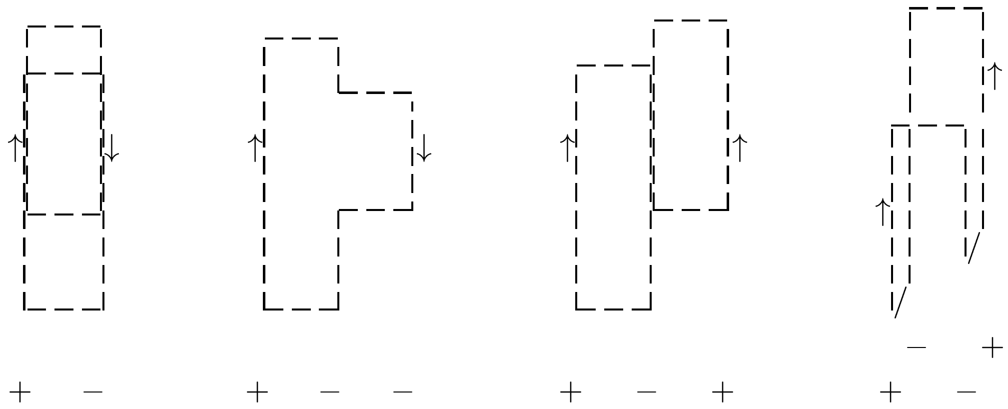
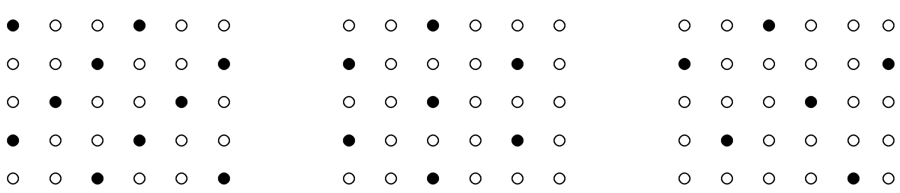


Fig. 2. Clusters with 4 jumps.



$\rho_n = 2/3$ $\rho_n = 3/4$ $\rho_n = 4/5$

Fig. 3. Ground state configurations at the order U^{-3} ($\bullet = -1$, $\circ = 1$).

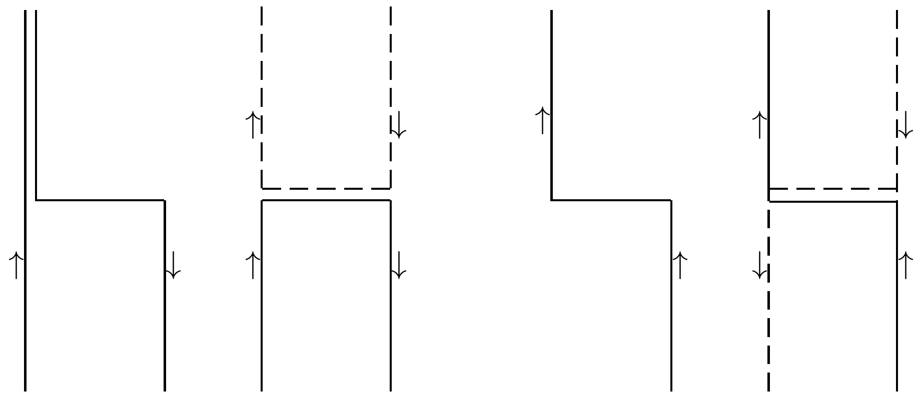


Fig. 4. From the trajectories to the circuits. The two represntative cases.