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THE FALICOV-KIMBALL MODEL, EFFECTIVE INTERACTION

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Abstract

The effective interaction between the static particles in the Falicov-Kimball model is studied, for large values of the coupling constant, using a convergent cluster expansion.

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1. Introduction

The Falicov-Kimball model consists of non-interacting spinless fermions, here called electrons, on a lattice. These particles move in a potential assuming the values $2U$ and 0 at each site, here interpreted as presence or absence of a classical nucleus. The density of these particles can vary and is controlled by the corresponding chemical potentials μ_n and μ_e. The hamiltonian of the system, on a finite d-dimensional cubic lattice $\Lambda \subset \mathcal{L} = \mathbb{Z}^d$, is

$$H = -k \sum_{(x,y)\subset\Lambda} c^+(x)c(y) + 2U \sum_{x\in\Lambda} w(x)c^+(x)c(x) \tag{1}$$

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 neighbor sites and k is the hopping coefficient. The variable $w(x)$ is 1 or 0 according to whether the site x is occupied or unoccupied by a nucleus. It is convenient to introduce also the spin variables $s(x) = 2w(x) - 1$ $\big(s(x) = \pm 1\big)$ to describe the nuclei configurations.

Let N_e and N_n denote the total numbers of electrons and nuclei

$$N_e = \sum_{x\in\Lambda} c^+(x)c(x) \ , \qquad N_n = \sum_{x\in\Lambda} w(x) \tag{2}$$

We consider the grand canonical ensemble specified by the density matrix

$$\rho = Z(\Lambda)^{-1} \exp\big(- \beta(H_\Lambda - \mu_e N_e - \mu_n N_n)\big) \tag{3}$$

with the partition function defined as

$$Z(\Lambda) = Z(\Lambda, \beta, \mu_e, \mu_n) = \sum_{\{w(x)\}} \mathrm{Tr}\ e^{-\beta(H_\Lambda - \mu_e N_e - \mu_n N_n)} \tag{4}$$

Here β is the inverse temperature, the sum is over all nuclei configurations with appropriate boundary conditions, and the trace is over the electron Fock space.

The Falicov-Kimball model was originally proposed [1] to describe a metal-insulator transition in solids. Later it was realized that it is also of interest to study the crystallization effect and as a simplified version of the Hubbard model [2]. The above description, in which the system is considered as a very simplified model for matter, corresponds to the second point of view.

We consider the case $U > 0$, though in this description the condition $U < 0$ would be more appropriate. Due to the symmetries of the model, both cases $U > 0$ and $U < 0$ are mathematically equivalent. Notice, however, that the half filled band condition $\rho_e + \rho_n = 1$, which plays a particular role in the case $U > 0$, corresponds to the neutrality condition $\rho_e = \rho_n$, in the case $U < 0$ (ρ_e and ρ_n are, respectively, the densities of the electrons and the nuclei). We remark that $0 \le \rho_e + \rho_n \le 2$.

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. 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 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 produces an effective interaction between the nuclei. This effective interaction energy can be defined by means of the grand canonical partition function

$$Z(\Lambda) = \sum_{\{s(x)\}} \exp\big(-\beta G_\Lambda(s)\big) \tag{5}$$

The effective interaction $G_\Lambda(s)$ can be rigorously determined with the help of a cluster expansion. This expansion follows from the Feynman-Kac or path integral representation of the system. Provided that the following condition is satisfied

$$U - |\mu_e - U| > 2d(1 + C_0)k \tag{6}$$

the cluster expansion is convergent. Here $C_0 > 0$ 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 convergence condition is satisfied. This interaction depends on the temperature. It will be studied here in the case in which temperature is sufficiently low (i.e., when $\beta > \beta_0$, where β_0 is some constant). All these constants are independent of $|\Lambda|$, the size of the system.

The cluster expansion gives the effective hamiltonian in terms of usual interaction potentials

$$G_\Lambda(s) = \sum_{A \subset \Lambda} \Phi_A(s_A) \tag{7}$$

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. 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 at low temperature (which depend on β), can be grouped in a term $\tilde{\Phi}_A$ of order $e^{-\beta U}$. The cluster expansion gives the main contributions to the interaction potentials $\Phi_A(s_A)$ expressed as a power series in the variable U^{-1}, and allows us (in principle) to compute these contributions at all orders. We remark that $\Phi_A \neq 0$ only if A is a connected set of sites (by paths going along nearest neighbors). Moreover, Φ_A is of order $U^{-(n-1)}$, if 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 $G_\Lambda(s)$ 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 the study a classical lattice system. Moreover, when a given approximation is considered one has, by means of the cluster expansion, a control on the terms neglected in the interaction.

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

$$G_\Lambda^{(1)}(s) = -\frac{1}{2}(\mu_n - \mu_e)\sum_x s(x) + \frac{k^2}{4U}\sum_{(x,y)} s(x)s(y) \tag{8}$$

Then, up to the order U^{-1}, the situation appears to be near to that of the antiferromagnetic Ising model in the presence of a external magnetic field. For the cubic lattice in dimension $d \geq 2$, we find 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 $\frac{1}{2}|\mu_n - \mu_e| < k^2U^{-1} - \eta$, where η is some positive quantity of order U^{-3}.

We recover then a result due to Lebowitz and Macris [3]. As noticed in ref. 3 the system is not exactly in the half filled band at positive temperature unless $\mu_e = U$. 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 up to order U^{-3} in the interaction potentials we find, for the square lattice ($d = 2$), the approximate hamiltonian

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

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]. 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 [6].

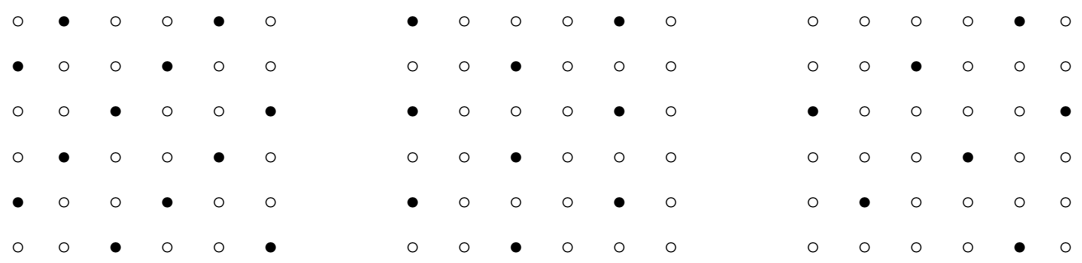

Fig. 1. Ground state configurations of densities 1/3, 1/4 and 1/5

The ground state configurations associated to the approximate hamiltonian $G_\Lambda^{(3)}(s)$ have also been examined in ref. 5 in the case of a square lattice ($d = 2$). Besides the chess board configurations for which the nuclei density is $\rho_n = 1/2$, three other kinds of periodic configurations with periods 3, 4 and 5 and having densities $\rho_n = 2/3$, $3/4$ and $4/5$, are found. These ground configurations are represented in Fig. 1.

Let $h = \frac{1}{2}(\mu_n - \mu_e)$ and assume that U is sufficiently large. Then, for

$$\begin{aligned} -h_1 < h < h_1 &= k^2U^{-1} - \frac{21}{4}k^4U^{-3}, \\ h_1 < h < h_2 &= k^2U^{-1} - 3k^4U^{-3}, \\ h_2 < h < h_3 &= k^2U^{-1} - k^4U^{-3}, \\ h_3 < h < h_4 &= k^2U^{-1} + \frac{1}{4}k^4U^{-3}, \end{aligned} \tag{10}$$

respectively, the mentioned configurations with densities $\rho_n = 1/2$, $2/3$, $3/4$ and $4/5$ are the only periodic ground configurations of the approximate hamiltonian. For $h > h_4$ the only periodic ground configuration is $s(x) = 1$ for all $x \in \Lambda$, with 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. A proof of these facts has been obtained [7] by continuing the analysis in ref. 5, where the ground state diagram was conjectured and partially proved.

We notice that Kennedy [8] has rigorously justified the existence of these periodic ground configurations for the Falicov-Kimball model, when U is sufficiently large, in a recent study of the ground states of this system at fixed densities. This work includes also several results for the system outside the half filled band.

We prove that the ground state configurations of the nuclei subsystem in the Falicov-Kimball model on a square lattice coincide with the above periodic configurations (for U sufficiently large and suitable values of μ_e). The associated phase diagram can be described in terms of the variable $h = (1/2)(\mu_n - \mu_e)$. The different domains where the configurations of densities $\rho_n = 1/2$ $1/3$, $1/4$, $1/5$, etc. are

proved to be the periodic ground states have lengths of order U^{-3} and are situated inside the corresponding intervals defined by Eq. 10. These domains are separated by small intervals whose length is of order U^{-5}. In order to investigate the ground state phase diagram inside these small intervals the next order terms in the nuclei 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. We finally remark that extensions of the present study to other kinds of lattices are possible along the same lines.

2. Path Integral Representation

In this section we study the Feynman-Kac or path integral representation for a system more general than the Falicov-Kimball model. This system is defined as follows. We consider on Λ, a finite box on the cubic lattice $\mathbb{Z}^d$, 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 site $x \in \Lambda$. We have the usual 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

$$H_\Lambda = -k_1 \sum_{|x-y|=1} c_1^*(x)c_1(y) - k_2 \sum_{|x-y|=1} c_2^*(x)c_2(y) + 2U \sum_x n_1(x)n_2(x) \tag{11}$$

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

In the expression of H_Λ the first two terms represent the kinetic energy H_0 and the last term is the potential energy V. The number operators $N_\sigma = \sum_x n_\sigma(x)$, with $\sigma = 1, 2$, 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 $N = |\Lambda|$ corresponds to the half filled band.

In order to develop the path integral representation 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. We

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

$$|X\rangle = c_1^*(x_1)\dots c_1^*(x_m)c_2^*(x_1')\dots c_2^*(x_n')|\emptyset\rangle \tag{12}$$

and remark that

$$V|X\rangle = v(X)|X\rangle \tag{13}$$

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

Let t be an integer variable, $0 \le t \le T$, which will be called the time. A trajectory $x = x(t)$ is defined as a sequence $x(0), x(1), \dots, x(T)$ 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 neighbor of $x(t)$. This last case we describe as a jump. A configuration of trajectories is a sequence

$$X(t) = (X_1(t), X_2(t)) = (x_1(t), ..., x_m(t); x_1'(t), ..., x_n'(t)) \tag{14}$$

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. In 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. 9).

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 $\exp(-H_\Lambda)$ asserts

$$\exp[-(H_0 + V)] = \lim_{T\to\infty} \left(\exp(-\frac{V}{T})(1 - \frac{H_0}{T})\right)^T \tag{15}$$

we get

$$\exp(-H_\Lambda)|X\rangle = \lim_{T\to\infty} \sum_{\Delta\in\mathcal{T}(\Lambda), X(0)=X} \exp\left(-\sum_{t=1}^{T} \frac{v(X(t))}{T}\right) \left(\frac{k_1}{T}\right)^{j_1(\Delta)} \left(\frac{k_2}{T}\right)^{j_2(\Delta)} |X(T)\rangle \tag{16}$$

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

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 the $(d+1)$-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

$$Z(\Lambda) = \mathrm{Tr}\exp(-H_\Lambda) \tag{17}$$

Because $\langle X(0)|X(T)\rangle \neq 0$ only if $\operatorname{supp} X_\sigma(0) = \operatorname{supp} X_\sigma(T)$, 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 $x \in \Lambda$. Then, we have $\langle X(0)|X(T)\rangle = (-1)^{\pi_1+\pi_2}$, where $(-1)^{\pi_\sigma}$ for $\sigma = 1, 2$ is the parity of the permutation $X_\sigma(0) \to X_\sigma(T)$.

3. Circuit Representation

In this section we describe a geometric representation equivalent to the path integral representation of section 2. Let a trajectory $x(0), x(1), \ldots, x(T)$ be represented by 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. For each $t = 0, 1, ..., T-1$ one of the following cases occurs:

(1) If $x \in \operatorname{supp} X_1(t) \backslash \operatorname{supp} X_2(t)$ 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 $x \in \operatorname{supp} X_2(t) \backslash \operatorname{supp} X_1(t)$ a trajectory with down-arrows goes along b and x is occupied by a particle with index $\sigma = 2$.
(3) If $x \in \operatorname{supp} X_1(t) \cap \operatorname{supp} X_2(t)$ two trajectories with opposite orientations intersect along b and x is occupied by two different particles.
(4) If $x \in \Lambda \backslash (\operatorname{supp} X_1(t) \cup \operatorname{supp} X_2(t))$ there is no trajectory on b and x is empty.

We represent these situations as follows: In case (1) we draw on the vertical bond $b \in \Omega^{per}$ 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. 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 also a dashed segment with an arrow in the direction of the jump.

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 some of the circuits may close by winding around the cylinder Ω^{per}. On the other side 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

$$\xi_0 = (x_0, t_0), \xi_1 = (x_1, t_1), ..., \xi_l = (x_l, t_l), \tag{18}$$

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 neighboring 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 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 has between t and $t+1$, multiplied by $2U$. Then, the contribution of a given circuit configuration to the operator $\exp(-H_\Lambda)$ is

$$\prod_\omega \exp(-\frac{U}{T}|\omega|) \left(\frac{k_1}{T}\right)^{j_1(\omega)} \left(\frac{k_2}{T}\right)^{j_2(\omega)} \prod_\omega{}' A(\omega), \tag{19}$$

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

$$\prod_\omega{}' A(\omega) = \mathcal{T} \prod_\omega \prod_{(\xi_i, \xi_{i+1}) \in J_1(\omega)} c_1^+(x_{i+1}) c_1(x_i) \prod_{(\xi_i, \xi_{i+1}) \in J_2(\omega)} c_2^+(x_{i+1}) c_2(x_i). \tag{20}$$

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 the 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.

We now apply the above analysis to the Falicov-Kimball model, which corresponds to the particular case in which the hopping coefficient k_1 equals zero. 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 if, and only if, for each vertical line (x, t) in the box Ω^{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 fix 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

$$Z(\Lambda) = \sum_{s \in Q(\Lambda)} Z(\Lambda, s) = \lim_{T \to \infty} \sum_{s \in Q(\Lambda)} \sum_{\{\omega_1, \ldots, \omega_r\}} \prod_{q=1}^{r} \exp(-\frac{U}{T}|\omega_q|) \left(\frac{k_2}{T}\right)^{j_2(\omega_q)} \alpha(\omega_q) \qquad (21)$$

where the last sum runs over all compatible families of oriented dashed circuits $\{\omega_1, \ldots, \omega_r\}$ 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.

This property can be proved as follows. We write, as indicated above, the product of creation and annihilation operators in chronological order (determined by the given configuration of dashed circuits). Let this product be $P = A_2 c^+(x_3) c(x_2) A_1 c^+(x_2) c(x_1)$, where $c^+(x_3), c(x_2), c^+(x_2), c(x_1)$ belong to the same circuit ω_1, the earliest. In A_1 and A_2 there are factors of the form $c^+(y)c(x)$ belonging or not to the circuit ω_1. However, and this is a first important observation, the point x_2 does not appear in A_1, since a vertical segment (with up arrows) of the circuit ω_1 connects $c(x_2)$ and $c^+(x_2)$. Therefore, $P = A_2 c^+(x_3) A_1 c(x_2) c^+(x_2) c(x_1) = A_2 c^+(x_3) A_1 (1 - n(x_2)) c(x_1)$. We next look for the operator $c(x_3)$ connected to $c^+(x_3)$ by a vertical segment in ω_1. It can be in A_1, for a down arrow segment, or in A_2, for an up arrow segment. Consider, for instance, the first case. Then, $P = A_2 c^+(x_3) A_1'' c^+(x_4) c(x_3) A_1' (1 - n(x_2)) c(x_1) = -A_2 A_1'' c^+(x_4) n(x_3) A_1' (1 - n(x_2)) c(x_1)$, again using the first observation. Now, some operators in A_1' may contain the point x_3. However, we always have $n(x_3) A_1' = A_1' n(x_3)$, since, and this is the second observation, every factor $c^+(x_3)$ is preceded by a factor $c(x_3)$ because all dashed segments have down arrows on the vertical line on the site x_3 (and $nc^+ = c^+(1-n), (1-n)c = cn$). Continuing this process we finally arrive at $P = B\alpha(\omega_1) \prod_y n(y) \prod_x (1 - n(x))$, where in B the operators which do not belong to the circuit ω_1 are left, in their initial order. The first product $\prod_y$ runs over all vertical down arrows segments and $\prod_x$ over all vertical up arrows segments of the circuit ω_1. The sign $\alpha(\omega_1) = \pm 1$ depends only on ω_1 because of the second observation, and the fact that all operators belonging to the other circuits appear in factors of the form $c^+(y)c(x)$ and have not moved in this process. This proves the factorization property for the sings.

It can be observed that, under the half filled condition, the weight of the dashed circuits decreases with U and with their length. Furthermore, the last for-

mula shows that, if the winding circuits were not present (for which this condition represents a global constraint), the system of oriented dashed circuits could be consider as a polymer system. In order to get rid of the constraint we consider the grand canonical ensemble. We therefore assume, as has been said in the Introduction, that $Z(\Lambda)$ represents the grand canonical partition function. Then, we have

$$Z(\Lambda, s) = \mathrm{Tr}\ \ e^{-\beta(H_\Lambda - \mu_e N_e - \mu_n N_n)}, \tag{22}$$

where the trace is taken over the electron Fock space. In order to find the expression of this new partition function the potential energy has to be modified to include the chemical potentials μ_n and μ_e.

Consider a vertical bond $b = [(x,t),(x,t+1)] \in \Omega^{per}$ and a given circuit configuration in Ω^{per}, compatible with the given classical configuration $s \in \Lambda$. As explained above, four situations 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 $b \in \Omega^{per}$ is

$$\begin{aligned}
\mu_n &= \frac{1}{2}(\mu_n + \mu_e) + \frac{1}{2}(\mu_n - \mu_e)s(x) \\
\mu_n &= \frac{1}{2}(\mu_n + \mu_e) + \frac{1}{2}(\mu_n - \mu_e)s(x) \\
\mu_n + \mu_e - 2U &= \frac{1}{2}(\mu_n + \mu_e) + \frac{1}{2}(\mu_n - \mu_e)s(x) + \mu_e - 2U \\
0 &= \frac{1}{2}(\mu_n + \mu_e) + \frac{1}{2}(\mu_n - \mu_e)s(x) - \mu_e
\end{aligned} \tag{23}$$

in cases (1) to (4), respectively. Therefore, if we write

$$Z(\Lambda, s) = \exp\big[\frac{1}{2}(\mu_n + \mu_e)|\Lambda| + \frac{1}{2}(\mu_n - \mu_e)\sum_{x\in\Lambda} s(x)\big]\ \tilde{Z}(\Lambda, s), \tag{24}$$

it turns out 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

$$\tilde{Z}(\Lambda, s) = \lim_{T\to\infty} \sum_{\{\omega_1,\ldots,\omega_r\}} \prod_{q=1}^{r} \exp(-\frac{\lambda(\omega_q)}{T}) \left(\frac{k}{T}\right)^{j(\omega_q)} \alpha(\omega_q) \tag{25}$$

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

$$\lambda(\omega) = U|\omega| \tag{26}$$

where $|\omega|$ is the length 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

$$\begin{aligned} &\lambda(\omega) = U\ell_1(\omega) - (\mu_e - 2U)\ell_2(\omega) \quad \text{or} \\ &\lambda(\omega) = U\ell_1(\omega) + \mu_e\ell_2(\omega) \end{aligned} \tag{27}$$

according to whether the circuit ω is going in the positive sense or in the negative sense.

4. The Nuclei Effective Interaction

In this section we introduce the cluster expansion which will allow us to determine the effective interaction for the nuclei subsystem in the Falicov-Kimball model.

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

$$\varphi_s(\omega) = \exp\left(-\frac{\lambda(\omega)}{T}\right)\left(-\frac{k}{T}\right)^{j(\omega)} \alpha(\omega), \tag{28}$$

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

$$\tilde{Z}(\Lambda, s) = \lim_{T\to\infty} \sum_{\theta\subset\Omega^{per}} \prod_{\omega\in\theta} \varphi_s(\omega) \tag{29}$$

where the sum runs over all admissible families of oriented dashed circuits.

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 ref. 10.

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 $|\theta| = \sum_\omega \theta(\omega)|\omega|$ and its total number of jumps by $j(\theta) = \sum_\omega \theta(\omega) j(\omega)$.

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 $\varphi_\sigma(\theta) = 0$ otherwise. One defines on $\mathcal{M}$ the truncated functions φ_s^C by

$$\varphi_s^C(\theta) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sum{}' \prod_{i=1}^{n} \varphi_s(\theta_i) \tag{30}$$

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 $\varphi_s^C(\theta) \neq 0$ then θ is connected as a set in $I\!R^d$. A second consequence is that

$$\tilde{Z}(\Lambda, s) = \lim_{T\to\infty} \exp(\sum_{\theta\subset\Omega^{per}} \varphi_s^C(\theta)) \tag{31}$$

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

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

Let us recall that

$$Z(\Lambda) = \sum_{s\in Q(\Lambda)} \mathrm{Tr}\ e^{-H_\Lambda + \mu_e N_e + \mu_n N_n} = e^{\frac{1}{2}(\mu_n+\mu_e)|\Lambda|} \sum_{s\in Q(\Lambda)} e^{-G_\Lambda(s)} \tag{32}$$

hence, from Eqs. 21, 24, 31, the effective interaction is given by

$$G_\Lambda(s) = -\frac{1}{2}(\mu_n - \mu_e) \sum_{x\in\Lambda} s(x) - \lim_{T\to\infty} \sum_{\theta\subset\Omega^{per}} \varphi_s^C(\theta) \tag{33}$$

The last sum is over the clusters θ of oriented dashed circuits 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). We notice that 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

$$G_\Lambda(s) = \sum_{A\subset\Lambda} \Phi_A(s_A) \tag{34}$$

Moreover, the interaction potentials $\Phi_A(s_A)$ are translation invariant. To see these facts we consider, for any cluster θ, the set $\pi(\theta) \subset \mathcal{L}$ 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 $\theta(\omega) \neq 0$). 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 neighbor sites). Then

$$\Phi_A(s_A) = \lim_{T\to\infty} \sum_{\theta:\pi(\theta)=A} \varphi_s^C(\theta), \tag{35}$$

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

$$\Phi_A^{(n)}(s_A) = \lim_{T\to\infty} \sum_{\substack{\theta:\pi(\theta)=A \\ j(\theta)=n}} \varphi_s^C(\theta). \tag{36}$$

From the above discussion 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 neighbors is a connected graph). Since the number of jumps $j(\theta)$ is always even (in a cubic lattice) $\Phi_A^{(n)} \neq 0$ only if n is an even number. Moreover, $\Phi_A^{(n)} \neq 0$ only if n is larger or equal than the smallest length which can have a closed path, along the bonds of A, passing 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}.

It is in this way, by means of Eq. 36, that the approximate hamiltonians at the orders U^{-1} and U^{-3}, whose expression was given in the Introduction (Eqs. 8 and 9), can be obtained. The hamiltonian $G_\Lambda^{(1)}$ comes from the contributions of the clusters with two jumps (which reduce to only one circuit). The next approximate hamiltonian $G_\Lambda^{(3)}$ is obtained by taking also into account the contributions of the clusters with four jumps. Only the contributions of the clusters made with non winding circuits are taken into account in these expressions and, furthermore, it is assumed that the clusters can be infinitely extended in the time direction. It is easily seen that the corrections due to this approximation are of order e^{-U}. However, in order to be able to apply the methods of classical statistical mechanics to the considered system, and to derive the results reported in the Introduction, one needs to estimate the remaining contributions, which have been neglected when considering the approximate hamiltonians. This can be done, again with the help of the cluster expansion. An explanation of this last point is given in the following section.

5. Convergence Properties

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

$$F_x(s) = \sum_{\theta : x \in \pi(\theta)} \varphi_s^C(\theta) \tag{37}$$

where the sum runs over all clusters whose projections $\pi(\theta)$ contain the site x. Among other properties 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 $\xi \in \Omega^{per}$ and under the appropriate conditions, the series

$$\sum_{\omega : \xi \in \omega} \varphi_s(\omega) \tag{38}$$

is absolutely convergent. We begin by considering the restriction of this sum to non-winding circuits. Such a circuit is described by the set of its vertices $\xi_0, \xi_1, \ldots, \xi_{2l} = \xi_0$, satisfying some conditions, with $\xi_q = (x_q, t_q) \in \Omega^{per}$. Let (ξ_0, ξ_1), (ξ_2, ξ_3),..., (ξ_{2l-2}, ξ_{2l-1}) be the vertical lines of ω, of lengths $m_i = |t_{2i-1} - t_{2i-2}|$, $i = 1, 2, ..., l$. Let (ξ_1, ξ_2), (ξ_3, ξ_4),..., (ξ_{2l-1}, ξ_{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 $\xi = (x, t) \in \Omega^{per}$ (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 $|\omega| = m_1 + m_2 + \ldots + m_l \ge m_1' + m_1'' + m_2 + \ldots + m_{l-1}$. 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. This choice gives at most $(2d)^l$ possibilities. As a consequence of these facts, we obtain

$$\begin{aligned}
\sum_{\xi \in \omega} |\varphi_s(\omega)| &= \sum_{\xi \in \omega} e^{-\frac{U}{T}|\omega|} (\frac{k}{T})^{j(\omega)} \\
&\le \sum_{l \ge 2} \frac{1}{T^l} \sum_{m_1', \ldots, m_{l-1}} e^{-\frac{U}{T}(m_1' + m_1'' + m_2 + \ldots + m_{l-1})} \, (2d)^l k^l \\
&\le \sum_{l \ge 2} \Big(\frac{1}{T} \sum_{m \ge 0} \exp(-\frac{U}{T} m) \Big)^l (2dk)^l
\end{aligned} \tag{39}$$

and, because

$$\frac{1}{T} \sum_{m \ge 0} \exp(-\frac{U}{T} m) = T^{-1} (1 - e^{-(U/T)})^{-1} \longrightarrow_{T \to \infty} 1/U \tag{40}$$

it follows that the sum converges if $U > 2dk$. More precisely, if $U/k \ge 2d(1 + a_1)$, 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.

As a consequence of these facts and of the general theory of cluster expansions, whose application to the present case is explained below, we obtain the following result: There exists a positive constant C_0, such that, if

$$U - |\mu_e - U| \geq 2d(1 + C_0)k \tag{41}$$

then, the series in the definition of the function $F_x(s)$ is absolutely convergent. Moreover, the sum of the absolute values can be bounded by $2dB_1k$, where B_1 is a constant.

We notice that C_0 is a number which can be computed from the theory. 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.

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

$$\sum_{x\in A} |\Phi_A(s_A)| \leq 2dB_1k \tag{42}$$

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

In order to prove these results we follow, as mentioned, the formalism of ref. 10. For simplicity in the exposition we take $\mu_e = U$. We introduce a new (positive) activity

$$\mu(\omega) = e^{-\frac{W}{T}|\omega|}\Big(\frac{\lambda}{T}\Big)^{j(\omega)} \tag{43}$$

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 $\varphi_s(\omega) = \varphi(\omega)$.

Observe that for the sum over the circuits containing a given point $\xi \in \Omega^{per}$, from Eq. 39, we have

$$\sum_{\xi\in\omega} \mu(\omega) \leq \Big(\frac{2d\lambda}{W}\Big)^2 \Big(1 - \Big(\frac{2d\lambda}{W}\Big)^2\Big)^{-1} \leq C_1^2 \tag{44}$$

provided that $W \geq C^{-1}2d\lambda$, with $C < 1$. Then $C_1^2 = C^2(1-C^2)^{-1}$. And, similarly, that for the sum over the circuits with a jump at a given point $\xi \in \Omega^{per}$, we have

$$\begin{aligned}\sum_{\xi\in J(\omega)} \mu(\omega) &\leq \sum_{l\geq 2} \sum_{m_1,m_2,\ldots,m_{l-1}} e^{-\frac{W}{T}(m_1+m_2+\ldots+m_{l-1})}\Big(\frac{\lambda}{T}\Big)^l \\ &\leq \sum_{l\geq 2} \Big(1 - e^{-\frac{W}{T}}\Big)^{-(l-1)} \Big(\frac{2d\lambda}{T}\Big)^l \leq \frac{W}{T} C_1^2\end{aligned} \tag{45}$$

under the same condition on W.

Next, we estimate the following sum

$$q(\omega_0) = \sum_S{}^* \mu(S) = \sum_S{}^* \prod_{\omega \in S} \mu(\omega) \tag{46}$$

extended to all sets S of circuits without intersections, such that all circuits in S intersect a given circuit ω_0.

Let $v_1, \ldots, v_{j_0}$ be the vertical lines of the circuit ω_0, whose number $j_0 = j(\omega_0)$ coincides with the number of jumps, and let $m_1^{(0)}, \ldots, m_{j_0}^{(0)}$ be their lengths. There can be 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, as in that of Eq. 44, we have

$$\sum_{v_1 \subset \omega}{}^* \mu(\omega) \leq C_1^2 \tag{47}$$

The other vertical lines in ω_0, such as say v_2, can be intersected by $0, 1, 2, \ldots$, etc. circuits. For each one of these circuits there is a jump at one point of v_2. 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

$$\begin{aligned} \sum_S{}^* \mu(S) &\leq \sum_{\nu_2}^{\infty} \sum_{\omega_1, \ldots, \omega_{\nu_2}}{}^* \mu(\omega_1) \ldots \mu(\omega_{\nu_2}) \\ &\leq \sum_{\nu_2}^{\infty} \binom{m_2^{(0)}}{\nu_2} \Big(\frac{2C_1^2 W}{T}\Big)^{\nu_2} \leq e^{\frac{m_2^{(0)}}{T} 2C_1^2 W} \end{aligned} \tag{48}$$

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

$$q(\omega_0) \leq \sum_{j_1=0}^{j_0} \binom{j_0}{j_1} C_1^{2j_1} e^{\frac{|\omega_0|}{T} 2C_1^2 W} \leq (1 + C_1^2)^{j(\omega_0)} e^{\frac{2C_1^2 W}{T} |\omega_0|} \tag{49}$$

Having established this property the discussion which follows is an easy adaptation of the method of ref. 10 (Section 4). One defines, associated to the Boltzmann factor $\varphi(X)$, the function

$$\Delta_X(Y) = (\varphi^{-1} \dot{D}_X \varphi)(Y) \tag{50}$$

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. 10, φ^{-1} is the inverse of φ in the sense of this product, and D_X is the derivation considered also in ref. 10. 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, where $\omega_0(\omega') = 1$ if $\omega' = \omega_0$ and 0 otherwise. We can write the following equation, for Y arbitrary and X without intersections,

$$\Delta_{\omega_0+X}(Y) = \varphi(\omega_0) \sum_{S \leq Y}^{*} (-1)^{N(S)} \Delta_{S+X}(Y - S) \tag{51}$$

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

$$I_m = \sup_{\substack{\omega_1,\ldots,\omega_n \\ m \geq n \geq 1}} \sum_{\substack{Y \\ N(Y)=m-n}} |\Delta_{\omega_1,\ldots,\omega_n}(Y)| \mu^{-1}(\omega_1) \ldots \mu^{-1}(\omega_n) \tag{52}$$

Then, using Eq. 51 and the bound on $q(\omega_0)$, one obtains

$$\begin{aligned}
\sum_{\substack{Y \\ N(X)+N(Y)=m}} & |\Delta_{\omega_0+X}(Y)| \mu^{-1}(\omega_0) \mu^{-1}(X) \\
& \leq |\varphi(\omega_0)| \mu^{-1}(\omega_0) \sum_{S \leq Y}^{*} |\Delta_{X+S}(Y - S)| \mu^{-1}(X) \\
& \leq I_m \ |\varphi(\omega_0)| \mu^{-1}(\omega_0) \sum_{S}^{*} \mu(S) \\
& \leq e^{-\frac{1}{T}(U - W - 2C_1^2 W)|\omega_0|} \Big(\frac{k(1 + C_1^2)}{\lambda} \Big)^{j(\omega_0)} \\
& \leq I_m r^m
\end{aligned} \tag{53}$$

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

$$U > 2dC^{-1}(1 + 2C_1^2)(1 + C_1^2) r^{-\frac{1}{2}} k = 2d(1 + C_0)k \tag{54}$$

That is, the condition in Eq. 41 (for $\mu_e = U$). If this condition is satisfied, we thus conclude that $I_{m+1} \leq I_m r$, for $m \geq 1$, and, because $I_1 = \sup_\omega |\varphi(\omega)| \mu^{-1}(\omega) \leq r$, we see that

$$I_m \leq r^m \tag{55}$$

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

$$\sum_X |\varphi^C(\omega + X)| \leq \sum_{m=1}^{\infty} \sum_{N(X)=m-1} |\Delta_\omega(X)| \leq \sum_{m=1}^{\infty} I_m \mu(\omega) \leq r(1 - r)^{-1} \mu(\omega) \tag{56}$$

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

$$\sum_{\xi \in X} |\varphi^C(X)| \leq r(1 - r)^{-1} \sum_{\xi \in \omega} \mu(\omega) \leq r(1 - r)^{-1} C_1^2 = B_0 \tag{57}$$

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

$$\sum_{x\in\pi(X)} |\varphi^C(X)| \leq r(1-r)^{-1}\frac{T}{2}\sum_{\xi\in J(\omega)} \mu(\omega) \leq r(1-r)^{-1}C_1^2 W = 2dB_1 k \tag{58}$$

Here ξ is any point in Ω^{per} such that $\pi(\xi) = x$. The constant B_1 can be written in terms of the previous constants using that $W = 2dC^{-1}\lambda$ and $\lambda = r^{-\frac{1}{2}}(1 + C_1^2)k$.

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

$$\begin{aligned} \sum_{\xi\in X} |\varphi^C(X)|R^{j(X)} &\leq B_0 \\ \sum_{x\in\pi(X)} |\varphi^C(X)|R^{j(X)-1} &\leq 2dB_1 k, \end{aligned} \tag{59}$$

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

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