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On Quantum Phase Transition. II. The Falicov–Kimball Model

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The Falicov–Kimball (FK) model[(1)] involves two types of interacting particles: first the itinerant spinless electrons are quantum particles, secondly the static ions are classical particles. It is striking to see that, despite the simplicity of its hamiltonian, the phase diagram of the FK model is highly sophisticated, moreover it remains in great part conjectural. An antiferromagnetic phase transition was proven for the FK model on a square lattice in the seminal paper of T. Kennedy and E. Lieb.[(2)] This result was extended by Lebowitz and Macris[(3)] to "small magnetic field." Then the same result was obtained by using a new method.[(4)] The main results of this paper concerns the two dimensional FK model on a square lattice, for which we apply the general results contained in ref. 5. First there exists an effective hamiltonian which is a long range many body Ising model, and which governs the behaviour of the ions. Secondly we compute explicitly the truncated effective hamiltonian up to the fourth order w.r.t. a small parameter (the inverse of the on site energy). Finally we use the classical Pirogov–Sinai theory, to get the hierarchy of the phase diagrams up to the fourth order. More precisely, we show that, when the chemical potential varies, the FK model exhibits, at low temperature, a sequence of phase transitions: first between phases of period two, then of period three, then of period four, and finally of period five. In each case the completeness of the phase diagram is proved. This paper supports the conjecture that the phase diagram of the FK model contains periodic phases outside of a Cantor set.

KEY WORDS: Falicov–Kimball model; itinerant electrons; phase transitions; Pirogov–Sinai theory; commensurate phases.

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1. INTRODUCTION AND RESULTS

The Falicov–Kimball (FK) model, which was introduced thirty years ago,[1] is a simple quantum lattice model. Despite its apparent simplicity its phase diagram is probably highly sophisticated. The model involves two types of interacting particles, first the itinerant spinless electrons are quantum particles, secondly the ions are classical particles. The FK model can be seen as a simplified Hubbard model, in which a specie of electrons does not move, and then become classical particles. Let us define the hamiltonian of the FK model:

$$\mathbf{H}_V = t \sum_{\langle x, y\rangle \in V} \{C_x^\star C_y + C_y^\star C_x\} + \frac{U}{2} \sum_{x\in V} \sigma(x)\,\tau(x) - \frac{\mu^i}{2} \sum_{x\in V} \sigma(x) - \frac{\mu^e}{2} \sum_{x\in V} \tau(x) \tag{1.1}$$

- $\langle \cdot, \cdot \rangle$ are the nearest neighbor sites.
- t is the hopping.
- U is the on site energy.
- μ_e and μ_i are the chemical potentials of the electrons and resp. of the ions.
- C_x^* (resp. C_x) are the fermionic creations (resp. annihilation) operators obeying to the Fermi statistic.
- $\tau_x = 2C_x^* C_x - 1$. $\sigma_a = +1$ if there is an ion at the site a and -1 otherwise.

On a bipartite lattice we have two symmetries: the electron to the non electron transformation $C_a^* \to C_a$, and the transformation $C_x \to -C_x$ on one part of the bipartite lattice. We can choose $U > 0$, because of the symmetries of the hamiltonian. It is convenient to use the parameters β for βt, U for $\frac{U}{t}$, μ^i for $\frac{\mu^i}{t}$, and μ^e for $\frac{\mu^e}{t}$.

In the recent years many papers have been devoted to the FK model. We first mention the seminal paper of T. Kennedy and E. Lieb,[2] in which an antiferromagnetic phase transition was proven. This result was extended by Lebowitz and Macris[3] to small "magnetic field" and then by Messager and Miracle Sole using a new method.[4] We mention the previous computations of the effective hamiltonian by Gruber *et al.*[7,8] The study of the ground states with higher periods goes back to Kennedy,[13] next to Watson,[18] Kennedy,[17] and Haller.[19] More generally, we refer to the review articles refs. 20 and 21 and to the references therein.

In this paper we mainly prove the existence, at low temperature, of three new domains in the plane $\{U^{-1} \times (\mu^e - \mu^i)\}$, in which a sequence of phase transitions between phases with the same periods occurs: first between phases of period three, then of period four and finally of period five. Next we describe how the approach contained in ref. 5, which is applied to the FK model. We noticed that, for $\mu^i = \mu^e = 0$, the classical part of the hamiltonian has an infinite degeneracy of ground states. The first main point contained in refs. 4 and 5 is to show that the quantum fluctuations remove the degeneration of the classical ground states leading to the coexistence of a finite number of phases. The second main point is the existence, at every temperature, of an effective hamiltonian, which is a long range many body Ising hamiltonian, via a convergent cluster expansion.[5] Notice that the notion of effective hamiltonian is implicit in ref. 5. Then we can use the deep results of the classical statistical mechanics such as the classical Pirogov–Sinai (P.S.) theory. Then the effective hamiltonian splits into two parts: the "truncated hamiltonian," which is computed explicitly up to the fourth order w.r.t. an expansion in U^{-1}, the remainder acts as a perturbation of the truncated hamiltonian, we notice that the fourth order effective hamiltonian was first computed in ref. 7. Then we get a hierarchy of refined phase diagrams for the FK model, together with the completeness of the phase diagram. The study of the FK model for other lattices and in higher dimension can be done as well, in particular the elaborated low temperature hierarchy of phase diagram of the triangular lattice FK model can be obtained from the results of ref. 9.

1.1. THE THERMODYNAMIC QUANTITIES

To define *the partition function, the free energy, the finite volume correlation functions*, we need the following definitions.

1.1.1. Definitions

- $\mathbf{\Sigma}_{\mathrm{V}}$ denotes the set of ions' configurations Σ_V
- $\mathscr{F}^f$ is the set of frozen electron's configurations F^f (non moving).

• The local algebra $\mathcal{O}$ is the tensor product of the local algebra built from the fermionic operators and from the commutative local algebra $\mathscr{S}$ built from the $\sigma(x)$,[9] a typical element is written $O \in \mathcal{O}$.

• An element of the *set of the boundary conditions* $\mathbf{\Sigma}_{\bar{\mathrm{V}}}$ in $\bar{V}$ is defined first by an ion's configuration $\Sigma_{\bar{V}} \in \mathbf{\Sigma}_{\bar{\mathrm{V}}}$, secondly we sum over the (classical) configurations of frozen electrons $F^f_{\bar{V}}$.

• The set of the finite volume correlation functions restricted to the subalgebra $\mathscr{S}$ with b.c. $\Sigma_{\bar{V}}$:

$$Z\{\Sigma_{\bar{V}}\} = \sum_{\Sigma_V} \operatorname{Tr}_{F_V \otimes F^f_{\bar{V}}} e^{-\beta H_V}$$

$$F(U, \mu^e, \mu^i) = -\lim_{V \to \infty} \frac{1}{\beta\,|V|} \ln Z\{\Sigma_{\bar{V}}\} \tag{0.4}$$

$$\left\langle \prod_{x \in X} \sigma(x) \right\rangle (\Sigma_{\bar{V}}) = \frac{\sum_{\Sigma_V} \operatorname{Tr}_{F_V \otimes F^f_{\bar{V}}} \{e^{-\beta H} \prod_{x \in X} \sigma(x)\}}{Z\{\Sigma_{\bar{V}}\}} \quad ()$$

The trace is over the Fock space defined in V, meanwhile $\Sigma_{\bar{V}}$ is fixed.

1.2. THE EFFECTIVE HAMILTONIAN

We have shown in ref. 5 for a wide class of models containing the FK model, the existence of an effective hamiltonian, which is a generalized Ising model $\mathscr{H}_\beta$ with long range and many body potentials. $\mathscr{H}_\beta$ is formally defined by:

$$Z\{H; \Sigma_{\bar{V}}\} = \sum_{\Sigma_V} [\operatorname{Tr}_{F_V \otimes F^f_{\bar{V}}} e^{-\beta H}] =: \sum_{\Sigma_V} e^{-\beta \mathscr{H}_\beta(\Sigma_V \mid \Sigma_{\bar{V}})}$$

The effective hamiltonian is well defined if the so called *S.I. condition*, is satisfied:

$$|\widetilde{\mu^e}| < \tilde{U} - 2v + h.o.$$

where $\widetilde{\mu^e} = A^{-1}.\mu^e$ and $\tilde{U} = A^{-1}.U$, where $A < 1$ is a positive constant, which will change along this paper.

We recall that $\mathscr{H}_\beta$ satisfies the following property: for any finite volume V, any set $X \in V$, and any ions' boundary condition $\Sigma_{\bar{V}} \in \mathbf{\Sigma}_{\bar{V}}$, the ionic correlation functions defined from H and the ionic conditional expectation functions defined w.r.t. $\mathscr{H}_\beta$ fulfill the following identities:

$$\left\langle \prod_{x \in X} \sigma_x \right\rangle^{\mathrm{H}} (\Sigma_{\bar{V}}) = E^{\mathscr{H}_\beta} \left[\prod_{x \in X} \sigma_x \,\middle|\, \Sigma_{\bar{V}} \right] \tag{1.2}$$

We define the set of the closed circuits $\mathscr{A}(Z^2)$ built on the square lattice Z^2, the edges of the circuits, which, in the case of the FK model, are the number of jumps, can have an arbitrary multiplicity. The effective hamiltonian $\mathscr{H}_\beta$ is defined via the potentials $\Psi^{\beta}[\Sigma_{\mathscr{A}}]$, which are real valued functions defined by the restriction of $(\Sigma_V \mid \Sigma_{\bar{V}})$ to the circuits $\mathscr{A}$:

$$\mathscr{H}_{\beta}(\Sigma_V \mid \Sigma_{\bar{V}}) = \sum_{\{\mathscr{A} \in \mathscr{A}(Z^2)\}} \Psi^{\beta}[\Sigma_{\mathscr{A}}]$$

We define the p order decomposition of the effective hamiltonian:

$$\mathscr{H}_{\beta}(V) = \mathscr{H}^{o}_{\beta}(V) + \cdots + \mathscr{H}^{p}_{\beta}(V) + \sum_{i=p+1}^{i=\infty} \mathscr{H}^{j}_{\beta}(V) =: \mathscr{H}^{\leqslant p}_{\beta}(V) + \mathscr{H}^{>p}_{\beta}(V)$$

where the p order truncated effective hamiltonian is defined by:

$$\mathscr{H}^{p}_{\beta}(\Sigma_V \mid \Sigma_{\bar{V}}) = \sum_{\{\mathscr{A} \in \mathscr{A}(Z^2) \mid |\mathscr{A}| = p\}} \Psi^{\beta}[\Sigma_{\mathscr{A}}]$$

The p order truncated effective hamiltonian depends explicitly of the temperature, the main problem is that the computations become rapidly complicated for large p. So it is convenient to define a new decomposition of $\mathscr{H}_{\beta}$, which is relevant at low temperature ONLY: the low temperature (L.T.) decomposition of $\mathscr{H}_{\beta}$, in which the truncated hamiltonians do not depend of the temperature. To do so, we split each potential in two parts:

$$\Psi^{\beta}[\Sigma_{\mathscr{A}}] =: \Psi^{\{\beta,\omega\}}[\Sigma_{\mathscr{A}}] + \Psi^{\infty}[\Sigma_{\mathscr{A}}]$$

The corresponding p order hamiltonians are $\mathscr{H}^{p}_{\{w,\beta\}}$ and resp. $\mathscr{H}^{p}_{\infty}$. Next the L.T. p order decomposition" is defined by: $\mathscr{H}_{\beta}$.

$$\mathscr{H}_{\beta}(V) = \mathscr{H}^{o}_{\infty}(V) + \cdots + \mathscr{H}^{p}_{\infty}(V) + \mathscr{H}_{\{w,\beta\}}(V) + \mathscr{H}^{>p}_{\beta}(V) \tag{1.3}$$

The crucial point, which is proved in ref. 5 is that, for β large, $\mathscr{H}_{\{w,\beta\}}(V)$ and $\mathscr{H}^{>p}_{\beta}$ act as perturbations of the hamiltonian $\mathscr{H}^{\leqslant p}_{\infty}$. This is the route, that we will follow to establish the hierarchy of the phase diagrams of the 2d. Falicov–Kimball model on a square lattice up to the fourth order.

Next we describe our main results. The first one is the computation of the fourth order L.T. decomposition of the effective hamiltonian by using the loop's formalism described in refs. 4 and 5.

1.3. Proposition: The L.T. Fourth Order Decomposition of the FK Model

We suppose an S.I. condition is satisfied.

(A) The hamiltonian **H** admits an effective hamiltonian $\mathscr{H}_{\beta}$ defined for every temperature.

(B) The hamiltonian $\mathscr{H}_\beta$ admits a L.T. fourth order decomposition:

(i) the zero order effective hamiltonian:

$$\mathscr{H}^{o}_{\infty}(V)=\frac{\mu^e-\mu^i}{2}\sum_{x\subset V}\sigma_x \tag{1.4}$$

(ii) The second order effective hamiltonian:

$$\mathscr{H}^{\leqslant 2}_{\infty}(V)=\frac{\mu^e-\mu^i}{2}\sum_{x\subset V}\sigma_x+\frac{1}{4U}\sum_{\{\langle x,\,y\rangle\cap V\neq\varnothing\}}\sigma_x\,.\,\sigma_y \tag{1.5}$$

(iii) the fourth order effective hamiltonian: ($\mathscr{P}_V$ is the set of plaquettes included in V)

$$\begin{aligned}\mathscr{H}^{\leqslant 4}_{\infty}(V)=\frac{\mu^e-\mu^i}{2}\sum_{x\subset V}\sigma_x&+\left[\frac{1}{4U}-\frac{9}{16U^3}\right]\sum_{\langle x,\,y\rangle\subset V\times V}\sigma_x\,.\,\sigma_y\\&+\frac{3}{16U^3}\sum_{\{(x,\,y)\cap V\neq\varnothing\,:\,|x-y|=\sqrt{2}\}}\sigma_x\,.\,\sigma_y\\&+\frac{1}{8U^3}\sum_{\{(x,\,y)\cap V\neq\varnothing\,:\,|x-y|=2\}}\sigma_x\,.\,\sigma_y\\&+\frac{5}{16U^3}\sum_{\{(x,\,y,\,z,\,t)\subset\mathscr{P}_V\,|\,(x,\,y,\,z,\,t)\cap V\neq\varnothing\}}\sigma_x\,.\,\sigma_y\,.\,\sigma_z\,.\,\sigma_t\end{aligned} \tag{1.6}$$

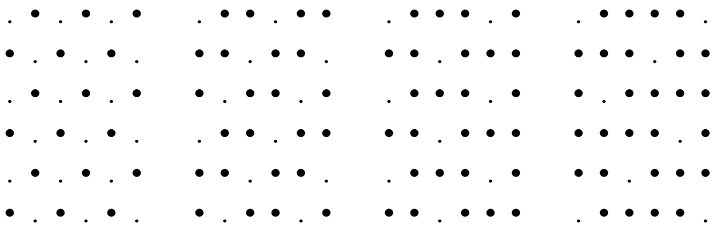
(iv) The tail potentials of the hamiltonian $\mathscr{H}^{>p}_{\beta}(V)$ and of $R_p^{\{\beta,\,\omega\}}[\Sigma_V\mid\Sigma_{\bar V}]$ decay like:

$$|\Psi^{\beta}[\Sigma_{\mathscr{A}}]|\leqslant\left\{\frac{1}{\tilde U-\widetilde{\mu^e}}\right\}^{(|\mathscr{A}|-1)};\qquad |R_p^{\{\beta,\,\omega\}}[\Sigma_V\mid\Sigma_{\bar V}]|\leqslant\left\{\frac{1}{\tilde U-\widetilde{\mu^e}}\right\}^{p} \tag{1.7}$$

1.4. The Hierarchy of the Phase Diagrams

1.4.1. *The Ground States of the Truncated Hamiltonians in the First Quadrant of $\{\mu^i-\mu^e,\frac{1}{U}\}$*

In the next figures we represent four ion's configurations. An ion is represented by a fat point, and the absence of an ion is represented by a point. The pure ion's configuration Σ^o is not depicted.



The origin is the lower left corner. Now the set of ground states is composed of five families $\hat{\Sigma}^{[r,q]}$ of ions' configurations, which are obtained by the composed actions of the shift T of the unit vector $(1,0)$, and of the rotation $R(\alpha)$ of angle α. The additional subscript is the order of the ground state. Notice that a ground state appearing at a given order, is a ground state for all the higher orders.

$q = o$. The family is reduced to the ion's configuration $\hat{\Sigma}^{[o,o]} \equiv \hat{\Sigma}^{[1,o]} \equiv \hat{\Sigma}^{[3,o]} = \Sigma^{o}$.

$q = \frac{1}{2}$. By mean of the action of T on $\Sigma^{\frac{1}{2}}$, we get: $\hat{\Sigma}^{[2,\frac{1}{2}]} \equiv \{\Sigma^{\frac{1}{2}}, \Sigma^{T(\frac{1}{2})}\}$

$q = \frac{1}{3}$. By mean of the composed actions of T and of $R = R[\frac{\Pi}{2}]$ on $\Sigma^{\frac{1}{3}}$, we get: $\hat{\Sigma}^{[4,\frac{1}{3}]} = \{\Sigma^{\frac{1}{3}}, \Sigma^{T(\frac{1}{3})}, \Sigma^{T^2(\frac{1}{3})}, \Sigma^{R\circ T(\frac{1}{3})}, \Sigma^{R\circ T(\frac{1}{3})}, \Sigma^{R\circ T^2(\frac{1}{3})}\}$

$q = \frac{1}{4}$. By mean of the composed actions of T and of $R = R[\frac{\Pi}{2}]$ on $\Sigma^{\frac{1}{4}}$, we get: $\hat{\Sigma}^{[4,\frac{1}{4}]} = \{\Sigma^{\frac{1}{4}}, \Sigma^{T[\frac{1}{4}]}, \Sigma^{T^2[\frac{1}{4}]}, \Sigma^{T^3[\frac{1}{4}]}; \Sigma^{R\circ T(\frac{1}{4})}, \Sigma^{R\circ T^2(\frac{1}{4})}, \Sigma^{R\circ T^2(\frac{1}{4})}, \Sigma^{R\circ T^3(\frac{1}{4})}\}$

$q = \frac{1}{5}$. By mean of the composed action of T and of $R' = R[\frac{\Pi}{3}]$ on $\Sigma^{[4,\frac{1}{5}]}$, we get: $\hat{\Sigma}^{[4,\frac{1}{5}]} = \{\Sigma^{\frac{1}{5}}, \Sigma^{T(\frac{1}{5})}, \Sigma^{T^2(\frac{1}{5})}, \Sigma^{T^3(\frac{1}{5})}, \Sigma^{T^4(\frac{1}{5})}; \Sigma^{[R'\circ(\frac{1}{5})}, \Sigma^{R'\circ T(\frac{1}{5})}, \Sigma^{R'\circ T^2(\frac{1}{5})}, \Sigma^{R'\circ T^3(\frac{1}{5})}, \Sigma^{R'\circ T^4(\frac{1}{5})}\}$

1.4.2. The Low Temperature Phase Diagrams of the Truncated Hamiltonians

(i) *The phase diagram of* $\mathscr{H}^{o}_{\infty}$ (Fig. 1). There is only one open domain $\mathscr{D}^{[0,0]}$ contained in the first quadrant Q. Along the line $L^{[0,1]}$ defined by $\mu^e = \mu^i$, every configuration is a ground state. There is only one low temperature phase, which is a small distortion of $\hat{\Sigma}^{[0,0]}$.

(ii) *The phase diagram of* $\mathscr{H}^{\leqslant 2}_{\infty}$ (Fig. 2). The two open disjoint domains $\mathscr{D}^{[2,0]}$, and $\mathscr{D}^{[2,\frac{1}{2}]}$ belongs to Q are separated by the line $L^{[2,1]}$ defined by: $|\mu^e - \mu^i| = \frac{2}{U}$ (Fig. 2). $\mathscr{H}^{\leqslant 2}_{\infty}$ has an infinity of ground states along $L^{[2,1]}$. The phases coexisting at low temperature in each one of the two domains are small distortions of the ground states $\hat{\Sigma}^{[2,0]}$, and resp. $\hat{\Sigma}^{[2,\frac{1}{2}]}$.

(iii) *The phase diagram of* $\mathscr{H}_{\infty}^{\leqslant 4}$ (Fig. 3). The five open disjoint domains $\mathscr{D}^{[4,0]}$, $\mathscr{D}^{[4,\frac{1}{2}]}$, $\mathscr{D}^{[4,\frac{1}{3}]}$, $\mathscr{D}^{[4,\frac{1}{4}]}$, $\mathscr{D}^{[4,\frac{1}{5}]}$ included in Q are separated by four curves $L^{[4,1]}$, $L^{[4,2]}$, $L^{[4,3]}$, $L^{[4,4]}$ defined in ref. 18 (Fig. 3). Along these curves $\mathscr{H}_{\infty}^{\leqslant 4}$ has an infinity of ground states. The phases coexisting at low temperature in each one of the five domains are small distortions of the ground states contained in the corresponding families $\hat{\Sigma}^{[4,0]}$, $\hat{\Sigma}^{[4,\frac{1}{2}]}$, $\hat{\Sigma}^{[4,\frac{1}{3}]}$, $\hat{\Sigma}^{[4,\frac{1}{4}]}$, $\hat{\Sigma}^{[4,\frac{1}{5}]}$.

Now we construct the hierarchy of the phase diagram of the FK model up to the fourth order. We recall that the "l shrinked domain" of B is defined by $B(l) =: \{x \in B \subset R^n \mid d(x, \bar{B}) < l\}$

• The zero order phase diagram of $\mathscr{H}_{\beta}$ and then of **H** is the phase diagram of $\mathscr{H}_{\infty}^{o}$ restricted to a shrinked domain. There is a "forbidden

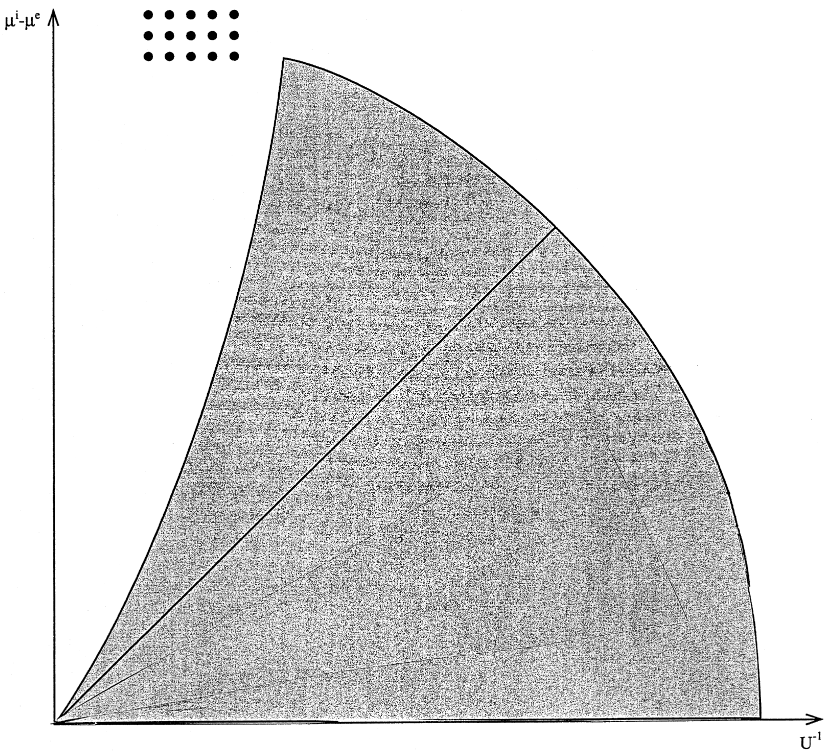


Fig. 1. Two phase diagrams: first the phase diagram of $\mathscr{H}_{\infty}^{o}$ is obtained by removing the shaded area to get the domain $\mathscr{D}_{o}^{o}$ in which $\mathscr{H}_{\infty}^{o}$ has a unique phase; secondly by looking at the full figure, we get the domain $\tilde{\mathscr{D}}_{o}^{o} \subset \mathscr{D}_{o}^{o}$, in which the phase diagram of $\mathscr{H}_{\infty}^{o}$ and then of **H** coincide. In the shaded area the phase diagram of **H** remains unknown at the zero order.

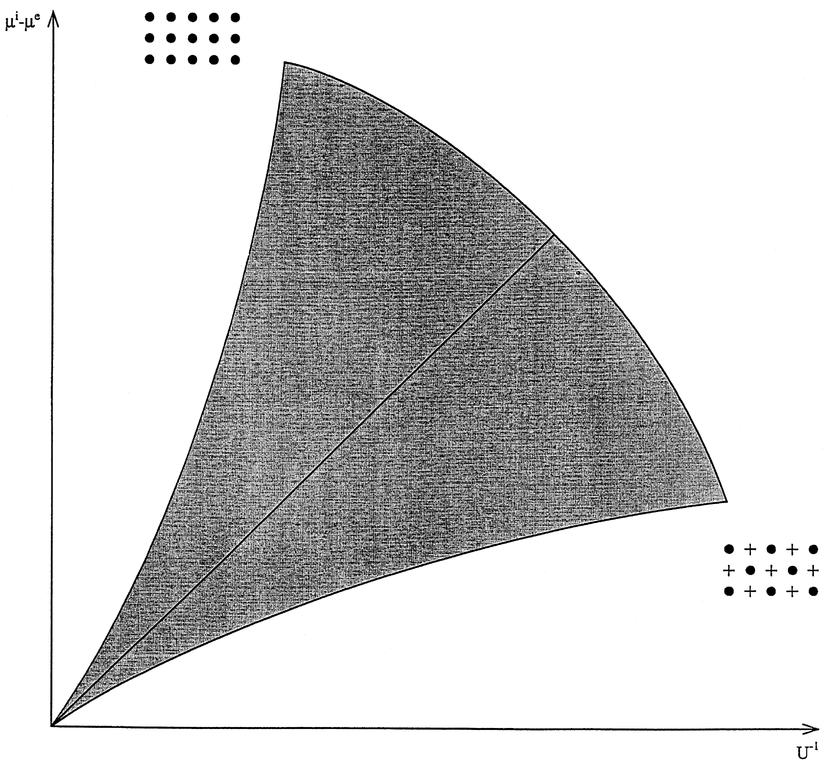


Fig. 2. Two phase diagrams: first the phase diagram of $\mathscr{H}_{\infty}^{\leqslant 2}$ is obtained by removing the shaded area, the quadrant is shared by the line $L^{[2,1]}$ into two domains $\mathscr{D}^2_{\frac{1}{2}}$, and $\mathscr{D}^2_o$, in which the stable phases have electron's density close to $\frac{1}{2}$, and 0; secondly by looking at the full figure, we get two shrinked domains $\widetilde{\mathscr{D}^2_{\frac{1}{2}}} \subset \mathscr{D}^2_{\frac{1}{2}}$, $\widetilde{\mathscr{D}^2_o} \subset \mathscr{D}^2_o$ in which the phase diagrams of $\mathscr{H}_{\infty}^{\leqslant 2}$ and then of **H** coincide. In the shaded areas the phase diagram of **H** remains unknown at the second order.

corridor" inherited from the tail potential, in which the phase diagram of $\mathscr{H}_\beta$ remains unknown (Fig. 1). We refine the phase diagram of $\mathscr{H}_\beta$ by considering $\mathscr{H}_{\infty}^{\leqslant 2}$.

- The second order phase diagram of $\mathscr{H}_\beta$ and then of **H** is the phase diagram of $\mathscr{H}_{\infty}^{\leqslant 2}$ in shrinked domains. We refine the phase diagram of $\mathscr{H}_\beta$ by considering $\mathscr{H}_{\infty}^{\leqslant 4}$.

- The fourth order phase diagram of $\mathscr{H}_\beta$ and then of **H** is the phase diagram of $\mathscr{H}_{\infty}^{\leqslant 4}$ in shrinked domains. Again appear "forbidden corridors" in which the phase diagram of $\mathscr{H}_\beta$ and then of **H** remains unknown (Fig. 4).

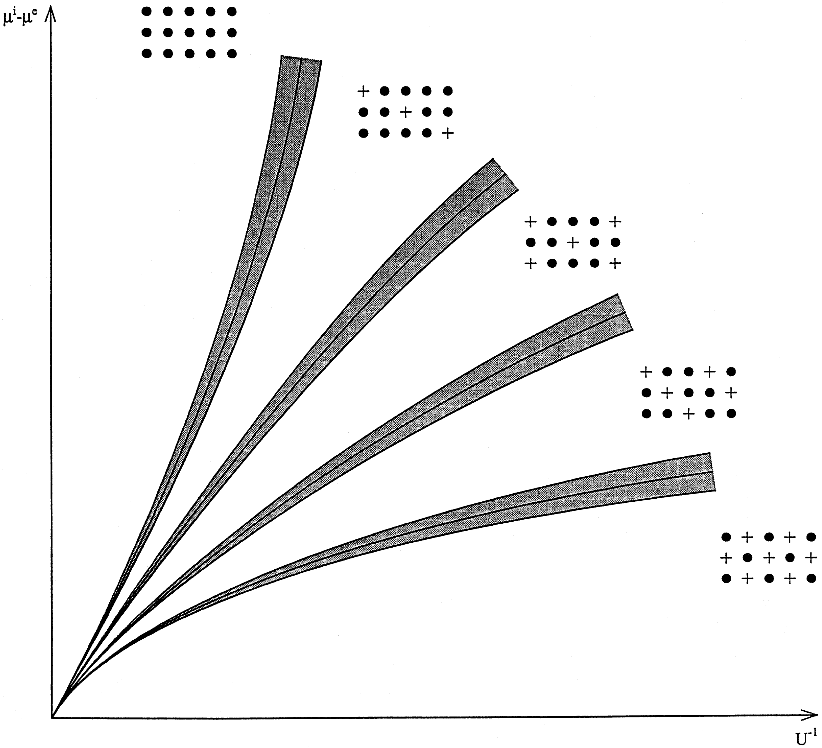


Fig. 3. Two phase diagrams: first the phase diagram of $\mathscr{H}_\infty^{\leqslant 4}$ is obtained by removing the shaded area, the quadrant is shared by the curves $L^{[4,1]}$, $L^{[4,2]}$, $L^{[4,3]}$, $L^{[4,4]}$ defined in ref. 18 into five domains $\mathscr{D}^4_{\frac{1}{2}}$, $\mathscr{D}^4_{\frac{1}{3}}$, $\mathscr{D}^4_{\frac{1}{4}}$, $\mathscr{D}^4_{\frac{1}{5}}$, D^4_o, in which the stable phases of $\mathscr{H}_\infty^{\leqslant 4}$ have electron's density close to $\frac{1}{2}$, $\frac{1}{3}$, $\frac{1}{4}$, $\frac{1}{5}$, and 0; secondly by looking at the full figure, we get five shrinked domains $\widetilde{\mathscr{D}^4_{\frac{1}{2}}} \subset \mathscr{D}^4_{\frac{1}{2}}$, $\widetilde{\mathscr{D}^4_{\frac{1}{3}}} \subset \mathscr{D}^4_{\frac{1}{3}}$, $\widetilde{\mathscr{D}^4_{\frac{1}{4}}} \subset \mathscr{D}^4_{\frac{1}{4}}$, $\widetilde{\mathscr{D}^4_{\frac{1}{5}}} \subset \mathscr{D}^4_{\frac{1}{5}}$, and $\widetilde{\mathscr{D}}^4_0 \subset \mathscr{D}^4_0$, in which the phase diagrams of $\mathscr{H}_\infty^{\leqslant 4}$ and then of **H** coincide. In the shaded areas the phase diagram of **H** remains unknown at the fourth order.

More generally we expect that the "forbidden corridors," appearing at a given order, are partly filled at the next order with higher periods phases separated by new "forbidden corridors," etc.

1.5. Theorem: The Hierarchy of the Phase Diagrams of the FK Model

The hamiltonian **H** satisfies an S.I. condition. Then there exists a set of strictly positive functions $A^{[r,s]}$ of $(\mu^e - \mu^i)$, such that the following properties hold.

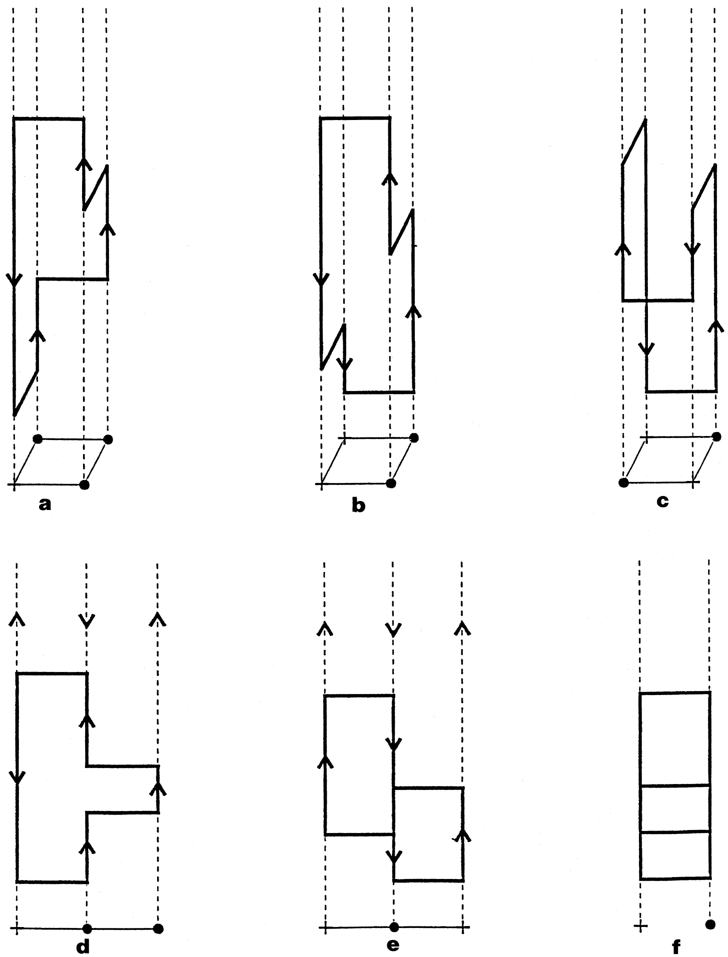


Fig. 4. Represents the differents loops involved in the computations of the potentials of the effective truncated hamiltonians of the FK model on the square lattice up to the fourth order.

(A) Phase transitions. Ergodic decomposition w.r.t. the ion's variables.

- Zero order. $\beta > A^{[o,o]}$

In the domain $\mathscr{D}^{[o,o]}(\frac{1}{U-|\mu^e|})$, there is uniqueness in the set of the periodic correlation functions.

- First order. $\beta > A^{[2,p]} \times U$.

(i) $p = o$. In the domain $\mathscr{D}^{[2,o]}(\frac{1}{[U-|\mu^e|]^3})$ there is uniqueness of the periodic correlation functions.

(ii) $p = \frac{1}{2}$. In the domain $\mathscr{D}^{[2,\frac{1}{2}]}(\frac{1}{[U-|\mu^e|]^3})$, there are two and only two extremal periodic correlation functions (pure phases).

- Third order. $\beta > A^{[4,q]} \times U^3$.

(i) $q = \frac{1}{2}$. In the domain $\mathscr{D}^{[4,\frac{1}{2}]}(\frac{1}{[U-|\mu^e|]^5})$, there are two and only two extremal periodic correlation functions.

(ii) $q = \frac{1}{3}$. In the domain $\mathscr{D}^{[4,\frac{1}{3}]}(\frac{1}{[U-|\mu^e|]^5})$, there are six and only six extremal periodic correlation functions.

(iii) $q = \frac{1}{4}$. In the domain $\mathscr{D}^{[4,\frac{1}{4}]}(\frac{1}{[U-|\mu^e|]^5})$, there are eight and only eight extremal periodic correlation functions.

(iv) $q = \frac{1}{5}$. In the domain $\mathscr{D}^{[4,\frac{1}{5}]}(\frac{1}{[U-|\mu^e|]^5})$, there are ten and only ten extremal correlation functions.

(v) $q = o$. In the domain $\mathscr{D}^{[4,o]}(\frac{1}{[U-\mu^e]^5})$, there is uniqueness of the periodic correlation functions.

Note.

- These results are extendable to the whole plane by using the symmetries of the hamiltonian.
- This hierarchical construction of the phase diagram suggests the existence of a devil's staircase phase diagram.
- We can expect also coexistence of phases of different periods.[18–20]

Content of the Paper. Chapter 2 contains:

- the computation of the effective hamiltonian up to the fourth order,
- the contour representation,
- the polymer expansion, and the cluster expansion,
- the Pirogov–Sinai theory which leads to the construction of the fourth order phase diagram of the FK model.

Chapter 3 is devoted to the completeness of the phase diagram.

2. THE PHASE DIAGRAM OF THE FALICOV–KIMBALL MODEL

The first step is to construct the L.T. fourth order decomposition of the FK hamiltonian. We compute explicitly the truncated effective hamiltonians up to the fourth order at $\beta = \infty$ by using the loop's representation contained in ref. 5. Notice that the computations are simpler if we use the formulas contained in refs. 7, 17, 18, and 19.

2.1. The Effective Hamiltonian

Each loop λ is endowed with a sign $\varepsilon(\lambda) = \{-1\}^{\pi(\lambda)}$. $\pi(\lambda)$ is the parity of the permutation between the incoming electrons and the outcoming electrons to the loop λ. $\phi^q_\infty(\Sigma_A)$ denotes the potential defined on the ion's configurations Σ_V restricted to the volume $A \subset V$, at the order q, computed for $\beta = \infty$.

2.1.1. The Zeroth Order Effective Potentials

$$\phi^o_\infty(\bullet) = h, \qquad \phi^o_\infty(-) = -h$$

2.1.2. The Second Order Effective Potentials

$$\phi^2_\infty(\bullet, \bullet) = 0, \qquad \phi^2_\infty(-, -) = 0;$$

$$\phi^2_\infty(\bullet, -) = \phi^2_\infty(-, \bullet) = -\int_0^\infty e^{-2sU}\, ds = -\frac{1}{2U}$$

In the first case a continuous non winding loop cannot be created. In the second case we sum over the s.d. of the non winding continuous loops of $\mathscr{L}_2$ (two jumps' non winding loop) created at a fixed time on a given bond, so that we have to integrate over the time between the two jumps.

2.1.3. The Fourth Order Effective Potentials

(a) The plaquette's potential with one electron or three electrons:

$$\varphi^4_\infty\begin{pmatrix} \bullet & \bullet \\ \bullet & - \end{pmatrix} = \varphi^4_\infty\begin{pmatrix} \bullet & \bullet \\ - & \bullet \end{pmatrix} = \varphi^4_\infty\begin{pmatrix} - & \bullet \\ \bullet & \bullet \end{pmatrix} = \varphi^4_\infty\begin{pmatrix} \bullet & - \\ \bullet & \bullet \end{pmatrix}$$

$$= \varphi^4_\infty\begin{pmatrix} - & - \\ - & \bullet \end{pmatrix} = \varphi^4_\infty\begin{pmatrix} - & - \\ \bullet & - \end{pmatrix} = \varphi^4_\infty\begin{pmatrix} \bullet & - \\ - & - \end{pmatrix}$$

$$= \varphi^4_\infty\begin{pmatrix} - & \bullet \\ - & - \end{pmatrix} = -\int_0^\infty e^{-2s_1U}\, ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3 = -\frac{2}{8U^3}$$

We have to integrate the signed densities built from the loops of $\mathscr{L}_4$ depicted in Fig. 4a. We integrate over the three times of occurrence of the successive jumps (the first jump is fixed). The parity of the permutation of the electrons is even so that the sign of the signed density is positive. The factor two arises from the fact that the electron can move at first in two directions.

(b) The plaquette's potential with two adjacent electrons:

$$\phi^4_\infty\begin{pmatrix} \bullet & \bullet \\ - & - \end{pmatrix} = \phi^4_\infty\begin{pmatrix} - & - \\ \bullet & \bullet \end{pmatrix} = \phi^4_\infty\begin{pmatrix} \bullet & - \\ \bullet & - \end{pmatrix} = \phi^4_\infty\begin{pmatrix} - & \bullet \\ - & \bullet \end{pmatrix}$$

$$= (-) \times (-) \int_0^\infty e^{-2s_1 U}\, ds_1 \int_0^\beta e^{-2s_2 U}\, ds_2 \int_0^{s_2} e^{-2s_3 U}\, ds_3 = \frac{4}{8U^3}$$

Again we integrate the signed densities built from the loops of $\mathcal{L}_4$ (four jumps' non winding loop) depicted in Fig. 4b. As the two electrons are permuted, the sign of the s.d. is negative. The factor four arises from the fact that the electrons have four different possibilities to move along the loop (two at first and then two after the first jump).

(c) The plaquette's potential with two opposite electrons:

$$\phi^4_\infty\begin{pmatrix} \bullet & - \\ - & \bullet \end{pmatrix} = \phi^4_\infty\begin{pmatrix} - & \bullet \\ \bullet & - \end{pmatrix}$$

$$= (-)^2\, 2 \int_0^\infty e^{-2s_1 U}\, ds_1 \int_0^{s_1} e^{-2s_2 U}\, ds_2 \int_0^{s_2} e^{+2s_3 U}\, ds_3 = \frac{4}{8U^3}$$

We integrate the signed densities built from the loops of $\mathcal{L}_4$ depicted in Fig. 4c over the times in between two consecutive jumps As the two electrons are permuted the sign of the signed density is negative. The origin of the entropical factor is that each one of the two electrons move in two directions.

The plaquette's potential with four electrons or with four ions:

$$\phi^4_\infty\begin{pmatrix} \bullet & \bullet \\ \bullet & \bullet \end{pmatrix} = \phi^4_\infty\begin{pmatrix} - & - \\ - & - \end{pmatrix} = 0$$

(d) The next nearest neighbor potential with two adjacent ions:

$$\phi^4_\infty\begin{pmatrix} & \bullet \\ - & \bullet \end{pmatrix} = \phi^4_\infty\begin{pmatrix} & - \\ \bullet & \bullet \end{pmatrix} = \phi^4_\infty\begin{pmatrix} & + \\ \bullet & + \end{pmatrix} = \phi^4_\infty\begin{pmatrix} & \bullet \\ + & + \end{pmatrix}$$

$$= \phi^4_\infty(\bullet, \bullet, -) = \phi^4_\infty(-, \bullet, \bullet) = \phi^4_\infty(\bullet, -, -) = \phi^4_\infty(-, -, \bullet)$$

$$= -\int_0^\infty e^{-2s_1 U}\, ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3 = -\frac{1}{8U^3}$$

We integrate the signed densities built from the loops of $\mathcal{L}_4$ depicted in Fig. 4d over the times in between two consecutive jumps. In both cases the sign is positive.

(e) The nearest neighbor potential with two non adjacent ions:

$$\phi^4_\infty\begin{pmatrix} & \bullet \\ \bullet & - \end{pmatrix} = \phi^4_\infty\begin{pmatrix} & - \\ - & \bullet \end{pmatrix} = \phi^4_\infty(\bullet, -, \bullet) = \phi^4_\infty(\bullet, -, \bullet)$$

$$\sim -\phi^4_\infty(\{\bullet, -\}, \{\bullet, -\})$$

$$= (-) \times (-) \int_0^\infty e^{-2s_1 U}\, ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3 = \frac{2}{8U^3}$$

These terms corresponds to the second order term of the cluster expansion, namely to the cluster, which is built from two intersecting loops of $\mathscr{L}_2$ (see Fig. 4e). Let us recall that this term has a negative sign in the cluster expansion.

(f) The two body nearest neighbor potential at the fourth order:

$$\phi^4_\infty(\bullet, -) = \phi^4_\infty(-, \bullet) =: (-) \times (-)\, \phi^4_\infty(\{\bullet, -\}, \{\bullet, -\}) = \frac{1}{8U^3}$$

We have computed the second order term occurring in the cluster expansion, where the clusters are composed of two intersecting loops of $\mathscr{L}_2$, which are located above the same bond (see Fig. 4f), this s.d. appears with a negative sign in the cluster expansion.

It is straightforward to rewrite the truncated hamiltonians in term of the σ_x r.v. to get the parts (i), (ii), and (iii) of Proposition 1.2. The part (iv) is proven in ref. 5 for a general class of models.

2.2. Phase Diagram of the Truncated Hamiltonians

In the next proposition, we describe the landscape of the ground states of the type $[r, q]$ in the first quadrant for the truncated effective hamiltonians $\mathscr{H}^o_\infty$, $\mathscr{H}^{\leqslant 2}_\infty$, and $\mathscr{H}^{\leqslant 4}_\infty$ established in ref. 17.

2.2.1. Proposition.[18]

(i) The ground state of $\mathscr{H}^o_\infty$ are, either the ion configuration $\Sigma^{[0,0]}$ in the domain $\mathscr{D}^{[0,0]}$, or infinitely many on the line $L^{[o,1]}$.

(ii) The ground states of $\mathscr{H}^{\leqslant 2}_\infty$ are either the ion configuration $\Sigma^{[2,0]}$ in the domain $\mathscr{D}^{[2,0]}$, or the two Neel configurations of $\hat{\Sigma}^{[2,\frac{1}{2}]}$ in the domain $\mathscr{D}^{[2,\frac{1}{2}]}$, or infinitely many on the line $L^{[1,1]}$.

(iii) The ground states of $\mathscr{H}^{\leqslant 4}_\infty$ are either the five families of configurations $\hat{\Sigma}^{[4,q]}$ (defined in the introduction) in the domains $\mathscr{D}^{[4,q]}$ ($q \in \{\frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}, 0\}$), or infinitely many on each curve $L^{[4,1]}$, $L^{[4,2]}$, $L^{[4,3]}$, $L^{[4,4]}$.

Proof. The zero order ground state is the pure ion configuration. The second orders are the two chessboard configurations of the Ising antiferromagnet. The fourth orders are defined on lattice blocks of size 3×3. Then a block is a ground state block of the class $[4, q]$ if it fits with the ground states defined by $\Sigma^{[4,q]}$ in the introduction. A part of the proposition was obtained in the papers of Gruber *et al.*[7,8] ∎

Notes. The ground states are indexed by their order despite they can be the same, because the local ground states are constructed from blocks of different sizes, at each order. For example the Neel local ground states are built from connected bonds at the second order, meanwhile they are built from 3×3 connected blocks at the fourth order. The inner boundaries and of the outer boundary of a contour are specified when it is needed. Next we define the contours of the type $[r, q]$.

2.2.2. The Contours of the Type [0, 0]

• In the domain $\mathscr{D}^{[0,0]}$, The contours of the type $[0, 0]$ are the the maximal connected sets of bonds which contain at most one ion per site.

2.2.3. The Contours of the Type [2, 0] and [2, $\frac{1}{2}$]

• In the domain $\mathscr{D}^{[2,0]}$ the contours of the type $[2, 0]$ are the the maximal connected sets of bonds with at most one ion per site.

• In the domain $\mathscr{D}^{[2,\frac{1}{2}]}$, the contours of the type $[2, \frac{1}{2}]$ are the antiferromagnetic contours, which are the connected dual lines to the bonds containing either two ions or no ion.

2.2.4. The Contours of the Type [4, $\frac{1}{2}$], [4, $\frac{1}{3}$], [4, $\frac{1}{4}$], [4, $\frac{1}{5}$], [4, 0]

The families of the third order contours are the corresponding maximal connected set of 3×3 bad blocks, defined successively in the domains $D^{[4,0]}$, $\mathscr{D}^{[4,\frac{1}{2}]}$, $\mathscr{D}^{[4,\frac{1}{3}]}$, $\mathscr{D}^{[4,\frac{1}{4}]}$, and $\mathscr{D}^{[4,\frac{1}{5}]}$.

2.2.5. The Contour Representation of the Partition Functions and the Correlation Functions of the Type [r, q]

• The boundary conditions in $\bar{V}$ are represented, in each domain $\mathscr{D}^{[r,q]}$, by two families of contours of the type $[r, q]$: a family of closed contours $\bar{\Gamma}^{[r,q]} = \{\bar{\gamma}_1^{[r,q]} \cdots \bar{\gamma}_n^{[r,q]}\}$ and, in general, a family of open contours $\bar{\Delta}^{[r,q]} = \{\bar{\delta}_1^{[r,q]} \cdots \bar{\delta}_m^{[r,q]}\}$. We will denote by $\varnothing^{[r,q]}$ the boundary conditions defined by the ground states of the type $[r, q]$.

• A configuration is given by two families of compatible contours of the type $[r, q]$, together with their inner and outer configurations: a family of closed contours $\Gamma^{[r,q]} = \{\gamma_1^{[r,q]} \cdots \gamma_i^{[r,q]}\}$ in V, and a family of open contours in V: $\Delta^{[r,q]} = \{\delta_1^{[r,q]} \cdots \delta_j^{[r,q]}\}$ compatible with $\bar{\Delta}^{[r,q]}$.

Now we define the rescaled conditional partition functions, the rescaled partition functions, and the contour correlation functions of the type $[r, q]$ with the b.c. $\bar{\Gamma}^{[r,q]}$ and $\bar{\Delta}^{[r,q]}$ in $\bar{V}$.

$$\Xi(\Gamma^{[r,q]}, \Delta^{[r,q]} \mid \bar{\Gamma}^{[r,q]}, \bar{\Delta}^{[r,q]}) = \frac{Z^{\mathscr{CONP}(\Gamma^{[r,q]}, \Delta^{[r,q]} \mid \bar{\Gamma}^{[r,q]}, \bar{\Delta}^{[r,q]})}}{Z_V^{\mathscr{CONP}(\overline{\varnothing^{[r,q]}} \mid \overline{\varnothing^{[r,q]}})}}$$

$$\Xi[\bar{\Gamma}^{[r,q]}, \bar{\Delta}^{[r,q]}] = \sum_{\{\Gamma^{[r,q]}, \Delta^{[r,q]}\}}^{*} \Xi(\Gamma^{[r,q]}, \Delta^{[r,q]} \mid \bar{\Gamma}^{[r,q]}, \bar{\Delta}^{[r,q]})$$

$$\rho(\{\gamma_1^{[r,q]}, \ldots, \gamma_k^{[r,q]}\} \mid \bar{\Gamma}^{[r,q]}, \bar{\Delta}^{[r,q]}) = \sum_{\{\Gamma^{[r,q]}, \Delta^{[r,q]}\} \mid \{\gamma_1^{[r,q]}, \ldots, \gamma_k^{[r,q]}\} \subset \Gamma^{[r,q]}\}}^{*} \Xi(\Gamma^{[r,q]}, \Delta^{[r,q]} \mid \bar{\Gamma}^{[r,q]}, \bar{\Delta}^{[r,q]})$$

The sum $*$ is the sum over the set of contours which are compatible with the boundary conditions $\{\bar{\Gamma}^{[r,q]}, \bar{\Delta}^{[r,q]}\}$.

2.2.6. Proposition: Peierls Estimates for the Truncated Hamiltonians

If an S.I. condition holds, there exists a family of functions $C^{[r,q]}$ of $\mu^e - \mu^i$, which go to zero when $\mu^e - \mu^i$ attains the boundary curves $L^{[r,q]}$ of the domains $\mathscr{D}^{[r,q]}$.

(i) The zero order. The contour's energy per bond is larger than $C^{[o,o]}$ in $\mathscr{D}^{[o,o]}$.

(ii) The second order. In the domain $\mathscr{D}^{[2,o]}$ the energy per unit bond of a contour is larger than $C^{[2,o]}$. In $\mathscr{D}^{[2,\frac{1}{2}]}$, the contour's energy per unit length of a contour is larger than $C^{[2,\frac{1}{2}]} \times \frac{1}{U}$.

(iii) The fourth order. In the domains $\mathscr{D}^{[4,q]}$, where q belongs to $[0, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}]$), the contour's energy per 3×3 block is larger than $C^{[4,q]} \times \frac{1}{U^3}$.

Proof. The zero order estimate is trivial. The first order estimate is the usual contour's energy per unit length of a contour of the antiferromagnetic Ising model with a magnetic field. Next we go to the fourth order. We deduce, from the Proposition 2.1.3, that every 3×3 block of a contour has an energy larger than $C^{[4,q]} \times \frac{1}{U^3}$. As we know, the proof of the Peierls condition is not automatic in this case, it is a consequence of ref. 17. ∎

2.3. The Contours' Cluster Expansions of the FK Model

We first convert the interacting contours into non interacting *decorated contours*.

2.3.1. The Decorated Contour Representation of the FK Model

The treatment of the different classes of contours of the type $[r, q]$ are analogous. We will treat only the third order, which is the most elaborated. We consider the case of the closed b.c. (the extension to arbitrary b.c. is easy). Following ref. 22, we introduce a cutoff $C[\beta, U-\mu^e]$, which shares the potentials into the "low energy" potentials and into the "high energy" potentials. $\Gamma = \{\gamma_1, ..., \gamma_p\}$ is a configuration of closed contours contained in V, we skip the reference to the type and to the class.

2.3.2. Definitions

We decompose the set of loops into two sets:

$$\mathscr{A}_{\{\geqslant C[\beta, U-\mu^e]\}} =: \{A \in \mathscr{A} \mid |A| \geqslant C[\beta, U-\mu^e]\}$$

$$\mathscr{A}_{\{< C[\beta, U-\mu^e]\}} =: \{A \in \mathscr{A} \mid |A| < C[\beta, U-\mu^e]\}$$

- A family $\Upsilon = \{v_1, ..., v_q\}$ of T. *contours* is built from the contours contained in Γ. We first define the thick contours, which are built by surrounding each contour $\gamma_j \subset \Gamma$ with a corridor of "width" $\frac{C[\beta, U-\mu^e]}{2}$ which contain the supports of the potential belonging to $\mathscr{A}_{\{< C[\beta, U-\mu^e]\}}$, secondly the subsets of the contours of Γ, which relative distance is smaller than $\frac{C[\beta, U-\mu^e]}{2}$, are glued together to build a T. contour v_i.
- $\mathscr{P}(\Upsilon)$ is the set of disjoint maximal partitions of the set of T. contours Υ. An element of $\mathscr{P}(\Upsilon)$ is written as $\{\Upsilon_{\alpha_1}, ..., \Upsilon_{\alpha_r}\}$.

The energy of a family of T. contours Υ is splitted into two parts:

$$\mathscr{H}_{< C[\beta, U-\mu^e]}(v_1, ..., v_p \mid \varnothing) = \sum_{j=1}^{j=q} \mathscr{H}^{\leqslant 4}(v_j) + \sum_{j=1}^{j=q} \sum_{\{A \in \mathscr{A}_{< C[\beta, U-\mu^e]} \mid A \cap v_j \neq \varnothing;\, |A| > 4\}} \Psi_A[v_j]$$

$$\mathscr{H}_{\geqslant C[\beta, U-\mu^e]}(v_1, ..., v_p \mid \varnothing) = \sum_{j=1}^{j=q} \sum_{\{A \in \mathscr{A}_{\geqslant C[\beta, U-\mu^e]} \mid A \cap v_j \neq \varnothing\}} \Psi_A[(v_1, ..., v_q)$$

- *A T. contour functional* is a functional of a T. contour v_j defined by:

$$\omega(v_j) = e^{-\beta \mathscr{H}_{\{< C[\beta, U-\mu^e]\}}(v_j)}$$

• *An interaction functional* is a functional of a family of T. contours $\{v_{r_1},\dots, v_{r_i})$ and of a set A which intersect the T. contours $\{v_{r_1},\dots, v_{r_i}\}$:

$$\eta_A(v_{r_1},\dots, v_{r_i}) = e^{\beta\Psi_A(v_{r_1},\dots,v_{r_i})} - 1; \qquad A \in \mathscr{A}_{\{\geqslant C[\beta, U-\mu^e]\}}$$

• *A decorated contour* $\Upsilon^{[r,p]} =: [\{v_1,\dots, v_r\}; \{A_1,\dots, A_p\}]$ is a maximal connected set. By connected, we mean that the supports of the T. contours $\{v_1,\dots, v_r\}$ and the supports of the sets $\{A_1,\dots, A_p\} \in \mathscr{A}_V$ are maximally connected.

Next we perform a new polymer expansion of the rescaled conditional partition functions by expanding the contour functionals and the interaction functionals defined above.

$$\Xi[\{v_1,\dots, v_p\} \mid \varnothing\}]$$
$$= \sum_{\{\Upsilon_{\alpha_1},\dots,\Upsilon_{\alpha_r}\}\subset \mathscr{P}(\Upsilon)} \left\{ \sum_{k=1}^{k=r} \left[\sum_{\{A_{k_1},\dots,A_{k_p}\}\subset P(A_V)} K_{\{A_{k_1},\dots,A_{k_p}\}}\{\Upsilon_{\alpha_k}\} \right]\right\}$$

with

$$K(\Upsilon^{[k,p]}) =: K_{\{A_{k_1},\dots,A_{k_p}\}}(\Upsilon_{\alpha_k}) = \prod_{i\in\alpha_k} \omega[v_i] \prod_{l=1}^{p} \eta_{A_{k_l}}[\Upsilon_{\alpha_k}]$$

Notes.

• The b.c. are now defined by a configuration of decorated contours $\bar\Upsilon^{[r,q]}$ and $\bar\Omega^{[r,q]}$ which supports are in $\bar V$. We define the rescaled partition function $\Xi(\bar\Upsilon^{[r,q]}\bar\Omega^{[r,q]})$ from the family of the rescaled conditional partition functions $\Xi(\Upsilon^{[r,q]}, \Omega^{[r,q]} \mid \bar\Upsilon^{[r,q]}\bar\Omega^{[r,q]})$.

• The main advantage of the polymer expansion written in term of decorated contours is that the decorated contours do not interact. Now we can perform a convergent C.E. of each rescaled partition function in term of its decorated contours.

2.3.3. Proposition: The Contours' Cluster Expansion

The hamiltonian **H** fullfill an S.I. condition. $\tilde C^{[q,r]}$ are the families of the functions of $\mu^e - \mu^i$ defined as in Proposition 2.2.4.

Then every partition function can be expanded into a family of convergent C.E. Each C.E. is performed for a family of contours, in the corresponding shrinked domains:

(i) $\mathscr{D}^{[o,o]}(\frac{1}{[r(U)-|r(\mu^e)|]})$, if $\beta > \tilde{C}^{[0,0]}$.

(ii) (a) $\mathscr{D}^{[2,0]}(\frac{1}{U^3})$, if $\beta > \tilde{C}^{[2,0]} \times U$; (b) $\mathscr{D}^{[2,\frac{1}{2}]}(\frac{1}{U^3})$, if $\beta > \tilde{C}^{[2,\frac{1}{2}]} \times U$.

(iii) (a) $\mathscr{D}^{[4,\frac{1}{2}]}(\frac{1}{[r(U)-|r(\mu^e)|]^5})$, if $\beta > \tilde{C}^{[4,\frac{1}{2}]} \times U^3$, (b) $\mathbf{D}^{[4,\frac{1}{3}]}(\frac{1}{[r(U)-|r(\mu^e)|]^5})$, if $\beta > \tilde{C}^{[4,\frac{1}{3}]} \times U^3$, (c) $\mathbf{D}^{[4,\frac{1}{4}]}(\frac{1}{[r(U)-|r(\mu^e)|]^5})$, if $\beta > \tilde{C}^{[4,\frac{1}{4}]} \times U^3$, (d) $\mathbf{D}^{[4,\frac{1}{5}]}(\frac{1}{[r(U)-|r(\mu^e)|]^5})$, if $\beta > \tilde{C}^{[4,\frac{1}{5}]} \times U^3$, (e) $\mathbf{D}^{[4,0]}(\frac{1}{[r(U)-|r(\mu^e)|]^5})$, if $\beta > \tilde{C}^{[4,0]} \times U^3$.

Proof. We refer to the Appendix of ref. 16 for a simple proof for the existence of a convergent C.E. ▮

2.4. Phase Transitions of the FK Model

We have shown in ref. 5 that the the classical PS theory[13] can be applied to the FK model if an S.I. condition is satisfied. Now we have to construct the phase diagram of the type $[r, q]$ of the FK model. The P.S. decompositions of $\mathscr{H}_\beta$ are obtained by varying the chemical potential. This construction is rather simple, because the ground states and the contours of a fixed type $[r, q]$ are obtained one from another by a geometric transformation. We will use the decorated contours of the type $[r, q]$, in place of the contours of the type $[r, q]$ of the corresponding truncated hamiltonians.

We choose to treat the case of the decorated contours of the type $[4, \frac{1}{3}]$. The other cases are similar or even simpler. In the domain $\mathscr{D}^{[4,\frac{1}{3}]}(\frac{1}{U^5})$ the hamiltonian $\mathscr{H}_\infty^{\leqslant 4}$ has six different ground states labeled by $p \in \{1, 2, 3, 4, 5, 6\}$. They are related one to another by the action of one the following six geometric transformations: $R^b[\frac{\pi}{2}] \circ S^a$ with $a \in \{0, 1, 2\}$, and $b \in \{0, 1\}$, which were defined in the introduction. As usually in the PS theory, we introduce *contour models*, which are six in our case. Each one is defined from a partition function, which b.c. is one of the six configurations contained in $\hat{\Sigma}^{[4,\frac{1}{3}]}$. We use for these b.c. the notations $\varnothing_p^{[4,\frac{1}{3}]}$, where $p \in \{1, 2, 3, 4, 5, 6\}$, which means the absence of contour in $\bar{V}$. We will skip the reference to the type. We start from the b.c. $\varnothing_{p_o}$. Let $\{\hat{v}_1, \dots, \hat{v}_r\}$ be the subset of the exterior contours of a given decorated contour configuration $\{\hat{v}_1, \dots, \hat{v}_r, \hat{v}_{r+1}, \dots, \hat{v}_n\}$. Each exterior contour generally contains several interiors. Each interior has itself an outer boundary, which configuration is one of the six ground states, say $\varnothing^{p_o}$. The six contour models are defined inductively through the six partition functions. Eachone is defined from the b.c. corresponding to one of the six ground states:

$$\Xi_V(\varnothing^p) = \prod_{i=1}^{i=r} K(\hat{v}_i) \frac{\Xi(\mathrm{Int}(\hat{v}_i) \mid \varnothing^{p_i})}{\Xi(\mathrm{Int}(\hat{v}_i) \mid \varnothing^{p_o})} \Xi(\mathrm{Int}(\hat{v}_i) \mid \varnothing^{p_o})$$

where $K(\hat{v}_i)$ is the weight of the exterior decorated contour $\hat{v}_i$. We define the new contour functionals for the decorated contour $\hat{v}_i$:

$$\Phi(\hat{v}_i) = K(\hat{v}_i)\,\frac{\Xi(\mathrm{Int}(\hat{v}_i) \mid \varnothing^{p_i})}{\Xi(\mathrm{Int}(\hat{v}_i) \mid \varnothing^{p_o})}$$

We obtain the six inductive presentations of the partition functions labeled by $p \in \{1, 2, 3, 4, 5, 6\}$.

$$\Xi_V(\varnothing^p) = \sum_{\hat{\Upsilon}p = \{\hat{v}_1,\ldots,\hat{v}_s\}} \prod_{i=1}^{i=s} \Phi(\hat{v}_i)$$

2.4.1. Proposition

The hamiltonian **H** satisfies an S.I. condition.

(i) There exists a positive function $\tilde{C}^{[2,\frac{1}{2}]}$ of $\mu^e - \mu^i$, such that for $\beta > \tilde{C}^{[2,\frac{1}{2}]} \times U$, the two Neel phases are stable in the domain $\mathscr{D}^{[2,\frac{1}{2}]}(\frac{1}{[U-|\mu^e|]^3})$,

(ii) There exists a set of positive functions $\tilde{C}^{[4,q]}$ of $\mu^e - \mu^i$, such that, for each $q \in \{\frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}\}$, the phases of family of the type $[4, q]$ are stable in the domains $\mathscr{D}^{[4,q]}(\frac{1}{[U-|\mu^e|]^5})$ for the corresponding values of $\beta > \tilde{C}^{[4,q]} \times U^3$.

Proof. As the proofs are similar for the contours of type $[r, q]$, we prove the stability for the phases for the type $[4, \frac{1}{3}]$ in the domain $\mathscr{D}^{[4,\frac{1}{3}]}(\frac{1}{[\tilde{U}-|\widetilde{r(\mu^e)}|]^5})$, which means that there exists a positive number $\tau^*_{\frac{1}{3}}$ such that, for large β, we have, for every couple of integers $\{s \neq t\}$, each one belonging to $\{1,\ldots, 6\}$:

$$\frac{\Xi(\mathrm{Int}(\hat{v}_i) \mid \varnothing^s)}{\Xi(\mathrm{Int}(\hat{v}_i) \mid \varnothing^t)} \leqslant e^{\tau^*_{\frac{1}{3}}\,\partial(\mathrm{Int}\,\hat{v}_i)}$$

This follows from the following fact: for any pair of partition functions defined in a finite volume V, the first one with b.c. $\varnothing^s$, the second one with b.c. $\varnothing^t$ $(s \neq t)$, there exists a couple of integers $[a, b]$, where $a \in \{0, 1, 2\}$, and $b \in \{0, 1\}$, such that:

$$\Xi(V \mid \varnothing^s) = \Xi(S^a \circ R^b_{\frac{\pi}{2}}[V] \mid \varnothing^t)$$

In other words, the decorated contours contained in V with the b.c. $\varnothing^s$, and the decorated contours contained in V, with the b.c. $\varnothing^t$ are related by the transformation $S^a \circ R^b\{\frac{\pi}{2}\}$ defined above. Two decorated contours appear in the two partition functions, if the transformed contours by $S^a \circ R^b\{\frac{\pi}{2}\}$ do not intersect ∂V. In other words, the difference between the two partition functions relies in the sum of the truncated functions defined on the clusters which, after the transformation $S^a \circ R^b[\frac{\pi}{2}]$, intersect ∂V. This sum is estimated by using the convergent C.E. of the Proposition 2.3.3. We first estimate the sum $\tau^*_{\frac{1}{3}}$ of the truncated functions computed for the clusters which intersect one point. Then we obtain:

$$\tau^*_{\frac{1}{3}} = \exp\left[-D_{[3,\frac{1}{3}]}\beta \frac{1}{[\tilde{U} - |\widetilde{\mu^e}|]^3} + h.o.\right]$$

where $D_{[3,\frac{1}{3}]}$ is a positive constant. This proves the stability of the phases.

The proof of the existence of the phase transitions of the type $[r, q]$ contained in the theorem is a consequence of the stability of the phases, shown in Proposition 2.4.2, see ref. 12. ∎

Note. As noticed above, we have used a simple version of the P.S. theory. We expect that the general P.S. theory will be needed in the case of phase transitions between phases with different periods to extend the results obtained for the ground states.(13, 18, 19)

3. ERGODIC DECOMPOSITION OF THE TYPE *[r, q]*

Next we establish the ergodic decomposition of the periodic correlation functions restricted to the algebra $\mathscr{S}$, we benefit of the standard methods of the classical statistical mechanics, which are applied to the effective hamiltonian $\mathscr{H}_\beta$. The ergodic decomposition of the periodic Gibbs states was first obtained in ref. 14 for the Ising model, and was extended to the framework of the PS theory in ref. 15. The case considered here of the FK model is simple because all the phases are stable in each domains under consideration. The ergodic decomposition will hold if the hypothesis contained in ref. 15 are satisfied. We first need an S.I. condition, and secondly that β belongs to the ranges of the phase coexistence, defined in Proposition 2.4.2, according to the domain $\mathscr{D}^{[r,q]}(\frac{1}{[\tilde{U} - |\widetilde{\mu^e}|]^{r+1}})$ that we consider. We give the main points of the proof, referring to ref. 14 and to ref. 15 for more details.

We start from a finite volume $V = L^2$. We use the decorated contours. A b.c. in $\bar{V}$ is generally represented by two families of decorated contours:

- a family of closed contours $\bar{\Upsilon}^{[r,q]}$,
- a family of open contours $\bar{\Omega}^{[r,q]}$.

Then a given contours' configuration in V, compatible with the b.c. is generally defined by two families of contours:

• a family of open decorated contours $\hat{\Omega}^{[r,q]} = \{\hat{\omega}_1^{[r,q]},..., \hat{\omega}_m^{[r,q]}\}$ compatible with $\bar{\Omega}^{[r,q]}$,

• a family of closed decorated contour $\hat{\Upsilon}^{[r,q]} = \{\hat{v}_1^{[r,q]},..., \hat{v}_n^{[r,q]}\}$.

Then the corresponding partition function is written as:

$$\Xi_V(\bar{\Upsilon}^{[r,q]}; \bar{\Omega}^{[r,q]}) = \sum_{\{\hat{\Upsilon}^{[r,q]};\, \hat{\Omega}^{[r,q]} \equiv \bar{\Omega}^{[r,q]}\}} \prod_{i=1}^{i=n} \prod_{j=1}^{j=m} \Phi(\hat{v}_i^{[r,q]})\, \Phi(\hat{\omega}_j^{[r,q]})$$

The open contours contained in V share the volume V into disconnected sub volumes $\{V_1^{p_1},..., V_{n+1}^{p_{n+1}}\}$, each one has an outer boundary configuration p_j, which is one of the ground states of type $[r, q]$.

$$\Xi_V(\bar{\Upsilon}^{[r,q]}; \bar{\Omega}^{[r,q]}) = \sum_{\{\hat{\Upsilon}^{[r,q]};\, \hat{\Omega}^{[r,q]} \bar{\Omega}^{[r,q]}\}} \prod_{i=1}^{i=m} K(\hat{\omega}_i^{[r,q]}) \prod_{j=1}^{j=n} \Xi_{V_i}(\varnothing_{p_j}^{[r,q]})$$

Now we define the periodic states as the infinite volume limit of the following average defined with respect to the period x^*:

$$\langle \sigma_X \rangle_V^{\text{per.}} = \frac{1}{L^2} \sum_{x^* \in V} \langle \sigma_{X+x^*} \rangle (\bar{\Upsilon}^{[r,q]}; \bar{\Omega}^{[r,q]})$$

Now we are left with a family of partition functions with b.c. corresponding to one ground state, say m_i, then we use the inductive contour representation given in the previous section for the partition functions with closed boundary conditions. Next we have to prove that, for all choice of boundary conditions, the following estimate is proven as in refs. 17 and 18:

$$\text{Prob}\left[\sum_{i=1}^{i=m} |\hat{\omega}_i^{[r,q]}| > L^{1+\delta} \right] < \varepsilon(L)$$

where δ is a positive number smaller than $\frac{1}{3}$, $\varepsilon(L)$ is a positive number going to zero when $L \to \infty$. To estimate the probability of the open contours, we use from one side the Peierls condition for the contours of the type $[r, q]$, and from the other side the stability condition to deduce the inequality:

$$\frac{\Xi(V_i \mid \varnothing_{m_i}^{[r,q]})}{\Xi(V_i \mid \varnothing_p^{[r,q]})} \leqslant e^{\tau_{r,q}^* \partial(V_i)}$$

These two estimates are both true in the corresponding ranges of β, which are defined in Proposition 2.3.2, for each domain $\mathscr{D}^{[r,q]}(\frac{1}{[\tilde{U} - \widetilde{|\mu^e|}]^{r+1}})$. The meaning of this estimate on the probability of the open contours is that the open contours occupy a small part of V, so we define the set of the "corridors" of width L^{δ} transverse to each open contours $\hat{\omega}_i^{[r,q]}$. Then these corridors have a total volume $L^{1+\delta}$, with probability close to one, for large L. The complements of these corridors define a new set of shrinked volumes $\{V_1^{p_1}(L^{\delta}),..., V_{n+1}^{p_{n+1}}(L^{\delta})\}$, some of which can be empty. The periodic correlations functions are obtained by a volume average over the correlation functions. The total contribution of the correlation functions, which supports are located in these corridors, goes to zero in the infinite volume limit. The remainder are the contributions of the correlation functions, which support are in the volumes $\{V_1^{p_1}(L^{\delta}),..., V_{n+1}^{p_{n+1}}(L^{\delta})\}$, far from the boundary. The correlation functions with support in each volume $V_1^{p_i}(L^{\delta})$ are the pure phases corresponding to the boundary m_i.[19] This means that, for every boundary condition defined by $\bar{\Upsilon}^{[r,q]}$, and by $\bar{\Omega}^{[r,q]}$, we produce the explicit ergodic decomposition of the periodic correlation functions, in the corresponding ranges of β, which were defined in Proposition 2.3.3, by computing the sum of volume $V_1^{p_i}(L^{\delta})$ with the same boundary condition m_i. At the zero order, there is only one extremal point in $\mathscr{D}^{[o,o]}(\frac{1}{\tilde{U}-|\mu^e|})$. At the second order there is only one extremal point in $\mathscr{D}^{[2,o]}(\frac{1}{[U-|\mu^e|]^3})$, and only two extremal points in $\mathscr{D}^{[2,\frac{1}{2}]}(\frac{1}{[U-|\mu^e|]^3})$. At the fourth order there is only one extremal point in $\mathscr{D}^{[4,o]}(\frac{1}{[U-|\mu^e|]^5})$, only two in $\mathscr{D}^{[4,\frac{1}{2}]}(\frac{1}{[\tilde{U}-|\widetilde{\mu^e}|]^5})$, six in $\mathscr{D}^{[4,\frac{1}{3}]}(\frac{1}{[U-|\mu^o|]^5})$, eight in $\mathscr{D}^{[4,\frac{1}{4}]}(\frac{1}{[U-|\mu^e|]^5})$, and ten in $\mathscr{D}^{[4,\frac{1}{5}]}(\frac{1}{[U-|\mu^e|]^5})$. This concludes the proof of the ergodic decomposition stated in Theorem 1.4.

Remark. From our families of convergent C.E. performed for the families of contour models, we can derived analyticity properties of the correlation functions which are expressed in term of the contours.

4. CONCLUSIONS

The existence of a cascade of new phase transitions, with higher periods is proved for the FK model. It is natural to dunk that, at least in part, the phase diagram is composed of periodic phases outside of a Cantor set. Watson, Kennedy and Haller have shown for the canonical ensemble the coexistenco of ground states of different periods[13, 18, 19] one should be able to extend this result at low temperature by using the equivalence of ensembles available in the classical statistical mechanics, together with the full P.S. theory. For $\mu^e = \mu^i = U$ and large values of $\frac{t}{U}$, T. Kennedy and E. Lieb were able to prove the existence of a first order phase transition. This result should be partly extendable to other values of the chemical potentials, despite we do not expect that the phases of higher periods should coexist. We point out the recent paper of Freericks, Lieb and Ueltschi,[23] who prove the segregation outside of the "half filled band." The problem of flux phases pointed out for the high T_c was partially solved, in the half filled band, for a wide class of models by E. Lieb in ref. 16. For the FK model coupled to a magnetic field, rational flux appear in some ground states only for small values of $\mu^i - \mu^e$, this was shown to be true for the ground states in ref. 9. Our approach is used to study the problem of the quantum interfaces in dimension three, in which the same structure appears. The quantum fluctuations select one dominant quantum interface. The 100 interface of the FK model (orthogonal to the vector 100) is rigid at low temperature due to the second order quantum fluctuations. The 111 interface is infinitely degenerate for the second order effective hamiltonian. The fourth order quantum fluctuations together with the Fermi statistic are responsible of the rigidity of the 111 interface at low temperature.[6]

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