The Falicov-Kimball model : a review of exact results and extensions

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THE FALICOV-KIMBALL MODEL: A REVIEW OF EXACT RESULTS AND EXTENSIONS

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Abstract

The Falicov-Kimball model is a simplified version of the the Hubbard model in which only one type of electron (e.g. spin down) is allowed to hop. It describes in particular a system of spinless quantum particles interacting with classical particles (Ising spins). In this review we present the progress which has been accomplished in the last decade concerning this model, with an emphasis on rigorous results. Our discussion includes the one, two, and three dimensional cases. We also show how certain techniques can be applied to other related models such as the static Holstein and Kondo models. Their common feature with the Falicov-Kimball model is that they consist of itinerant spinless electrons interacting with a classical field, associated with either a discrete Ising spin, a continuous scalar spin or a vector field. Finally we discuss a generalized Falicov-Kimball model of spin one-half electrons with on-site Hubbard interaction and interacting also with classical particles, as well as different models where the fermions are replaced by hard-core bosons. For the last class of models the interactions are truly many body but a limited number of rigorous results can be obtained using reflection positivity. The main issues discussed in this review concern the structure of ground states for the classical particles, and how they are affected by magnetic fluxes (via orbital coupling) and quantum statistics. Perturbative as well as non perturbative methods are used.

1. INTRODUCTION

Phase diagrams of quantum statistical lattice models are much less understood than their classical counterpart. In the quantum case, because of quantum fluctuations, not only the low temperature properties are difficult to extract but also the ground state behaviour. Recently much interest has been devoted to models of interacting (or "correlated") itinerant electrons. A prototypical system of this type is the twentyfive year old Hubbard model where spin one-half electrons hop on the sites of a lattice Λ and interact when they are on the same site. The hamiltonian is in second quantization (see sect. 2 for the notation)

$$H = - \sum_{x,y \in \Lambda, \sigma = \uparrow, \downarrow} t_{xy}^{(\sigma)} a_{x\sigma}^{\dagger} a_{y\sigma} + U \sum_{x \in \Lambda} (a_{x\uparrow}^{\dagger} a_{x\uparrow} - \frac{1}{2})(a_{x\downarrow}^{\dagger} a_{x\downarrow} - \frac{1}{2}) \qquad (1.1)$$

The usual Hubbard model corresponds to $t_{xy}^{(\uparrow)} = t_{xy}^{(\downarrow)} = t_{xy}$. Initialy it was introduced to discuss metal-insulator transitions and itinerant magnetism [1,2]. In this case U is positive, which corresponds to a repulsive on-site interaction between electrons favoring local magnetic moments. More recently it was thought to be a good candidate to understand high temperature superconductivity (again with $U > 0$). Although the investigations have not fulfilled all the expectations, it remains a very important model to describe strong electron correlations. Rigorous results concerning (1.1) are rather few and we refer to [3] for a recent review (see also [4] for a review of the Hubbard model and its generalisations).

A much more tractable model, which is the subject of this paper, is the so called Falicov-Kimball model (FK), which corresponds to $t_{xy}^{(\uparrow)} = 0$, $t_{xy}^{(\downarrow)} = t_{xy}$ with either $U > 0$ (repulsion) or $U < 0$ (attraction). In this model only one type of particle hops while the other one can be considered classical. In other words we have a family of hamiltonians depending on a configuration of classical particles $\{a_{x\uparrow}^{\dagger} a_{x\uparrow} = n_x^{cl}\}$ with $n_x^{cl} = 1$ or 0. For a given configuration $\{n_x^{cl}\}$ we have to solve a one electron problem in an external potential, but of course one allows the configuration of classical particles to vary, which makes the analysis highly non trivial. One can hope that a good understanding of this simpler model might lead to new insights for the Hubbard model.

The interpretations given to the FK model, and the motivations to study it, are quite diverse. Roughly speaking they fall into four categories that we descibe in the four paragraphs below.

It was first considered by Hubbard [1] and Gutzwiller [2] as a mathematical simplification of the Hubbard model (1.1), and thus it is sometimes refered to as "simplified Hubbard model". Another very interesting and more recent interpretation of the FK model is related to a Hubbard hamiltonian in which the hopping term of (1.1) is replaced by

$$\sum_{x,y\in\Lambda,\sigma,\sigma'\in\uparrow,\downarrow} t_{xy} a^{\dagger}_{x\sigma} a_{y\sigma'} \qquad (2.1)$$

which allows for hopping processes with spin flip. This model, introduced by Montorsi and Rasetti [5] can be shown to be equivalent to the FK model (see [4] for a review). An exact solution for this model was proposed in [5], but was shown later to be incorrect [6, 7].

Falicov and Kimball [8] introduced the model* to investigate metal-insulator transitions in mixed valence compounds of rare earth and transition metal oxydes [9]. These transitions are thought to have a purely electronic origin and the static particles are interpreted as $f-$ electrons, while the itinerant ones correspond to the $d-$ electrons of the conduction band. Later it was again considered to investigate ordering in mixed valence systems and binary alloys [10-13].

The model was reinvented by Kennedy and Lieb [14,15] as a very primitive model of matter to study crystalization and was called "static Hubbard model". In this interpretation the classical particles are thought of as ions and the fermions as spinless electrons. Relevant questions concern for example the formation of atoms, molecules, crystals.

Here we introduce a fourth point of view. One can view the FK model as a special case of a more general class of models where the electrons interact with a classical field. If this field is a discrete spin variable taking values ± 1 we recover the usual model. If it is a continuous scalar variable representing the configuration of classical oscillators we have the static Holstein model which is used to study electron-phonon interactions in molecular crystals. In this framework one can discuss the Peierls instability. When the classical field is vectorial we can interpret the model as a static lattice Kondo model. The vector field then models the spin of the impurities. If furthermore the amplitude of this vector field is allowed to vary we get a model which is equivalent to the Hubbard model in the

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* The original model of Falicov and Kimball in [8] has extra complications.

Hartree-Fock approximation. Relevant questions then concern the ordering of the vector field, i.e. ferromagnetic, antiferomagnetic order and continuous symmetry breaking.

Let us recall that one of the great achievements of classical statistical mechanics was to show that a single two body potential is able to produce a variety of different phases from the gazeous up to the crystaline as one increases the density. However this two body potential has to be injected by hand in the theory and is usually chosen to be independent of the density and temperature of the system. In reality the forces between atoms, molecules, or magnetic impurities, have a more microscopic origin in quantum mechanics: they arise from the subtle combination of the Coulomb potential and the Pauli principle. The two body potential of classical statistical mechanics should really be considered as an effective potential, depending on the density and temperature. A priori it is not even clear that such a potential is a well defined notion. In the FK model one can adress the question of defining and calculating this potential in some regimes of density and temperature.

In this paper we review rigorous results obtained in recent years. We have also included some material which has not appeared in the literature, although ideas and techniques are certainly not completely original (sect. 5 and 6).

Let us briefly mention aspects that are beyond the scope of this paper. Many results which we shall not discuss were obtained using exact diagonalisation and quantum Monte Carlo methods (see [4,16,17]). The exact solution of the FK model in the limit of high dimension $d \to \infty$ [18] has been found [19–22]. In analogy with spin lattice models a mean field hamiltonian which becomes exact in the limit $d = \infty$ has been considered [23, 24]. Furthermore an argument has been proposed [13] suggesting that the phase diagram for the two dimensional FK model should be qualitatively the same as for $d = \infty$. Several authors have also considered mean field methods and the limit of high dimensionality (e.g. [13], [25–29]). Other extensions which we do not discuss here are, the FK model with long range hopping [30], the spin 1/2 FK model [31,32], and the FK model in the continuum [33].

The first rigorous results were obtained by Kennedy and Lieb [14,15], and independently, by Brandt and Schmidt [12], for systems on bipartite lattices at the symmetry point (half-filled band). They proved that at low temperatures the ions tend to arrange them-

selves on one sublattice, therefore forming a crystal. These results were then extended by Lebowitz and Macris [34] to a domain of chemical potentials around the symmetry point. It was pointed out in [14] that the Pauli principle is important to get a crystaline state since this state cannot be obtained if one replaces fermions by ordinary bosons. However we show that *hard-core* bosons can produce a crystaline state, so that an on site repulsion in real space is sufficient.

Other rigorous results which will be discussed in the following sections concern the *one dimensional* ground state phase diagram [13, 35–48], the question of segregation [36,39,43,49], and general properties of the one-dimensional system [16,46,50–52]. The *two dimensional* model is much more difficult because there is no analytical expression for the total energy of periodic configurations (see [50,51] for one dimension). General properties of the phase diagram have been obtained on the square lattice [16,34,35,37,53–57], and on the triangular lattice [55]. Furthermore in the case of two dimensional systems an interesting question is related to the so-called "flux phase conjecture" and this was investigated both for bipartite lattices and for the triangular one [55,58].

The paper is organised as follows. In section 2 we give a precise definition of the model, the ground state energy, the effective potential, and dicuss symmetries. The zero temperature phase diagram in one dimension is described in section 3. Section 4 concerns the two and three dimensional cases. There we review some basic theorems of Kennedy and Lieb which are non perturbative in the sense that the method of proof does not involve perturbation theory and the results hold for all U. These concern only the half-filled band however. We also give more detailled information for other fillings, and large U, and discuss the flux phase problem. The low temperature phase diagram is discussed for densities close to one-half. Section 5 concerns results on interacting systems. We discuss spin one-half fermions (with Hubbard interaction) as well as hard-core bosons. We explain how to use reflection positivity techniques to get information on the ground state of the half-filled band for all U. For the case of hard-core bosons we also give results valid for other fillings, but they are limited to large U. Section 6 deals with the static Holstein and lattice Kondo models. We discuss the finite temperature behaviour of the Holstein model for densities close to one-half, and the ground state of the static Kondo model at half filling.

2. THE MODEL AND MAIN DEFINITIONS

The systems under investigation consist of identical quantum particles on a finite, but arbitrary, d dimensional lattice $\Lambda = \{x\}$, with vertices x in $\mathbf{R}^d$, together with a family $\mathcal{B} = \{(x, y)\}$ of bonds $(x, y) \subset \Lambda$ describing the allowed hoppings of the particles on the lattice. The number of vertices is $|\Lambda|$. We shall always assume that the lattice is connected. Most of the time we shall be concerned with regular, periodic lattices, such as a cubic lattice $\Lambda \subset \mathbf{Z}^d$ with $\mathcal{B}$ the bonds formed by nearest neighbours $< xy >$, but some statements hold more generally*.

To introduce the kinetic energy of the particles, we associate with the lattice a $|\Lambda| \times |\Lambda|$ complex, hermitian, matrix T with elements t_{xy}, with x and y in Λ,

$$t_{xy} = t_{yx}^* = |t_{xy}|e^{i\theta_{xy}}, \qquad \theta_{xy} = -\theta_{yx} \tag{2.1}$$

such that $t_{xy} = 0$ if $(x, y) \notin \mathcal{B}$. When $\Lambda \in \mathbf{Z}^d$ the matrix elements are non vanishing only for nearest neighbour sites (unless specified otherwise) and are sometimes denoted by $t_{<xy>}$.

In the framework of the tight binding approximation t_{xy} is related to the matrix element of the Laplacian between atomic orbitals localised around x and y, and is alternatively called overlap, transfer integral, hopping. We adopt the last terminology. If the hoppings are real they can have any sign and if they are complex the phase usually models the orbital coupling of the electrons to a magnetic field. One can think of the phase θ_{xy} as the integral of a vector potential $\int_x^y A.dl$ along the bond (x, y) of $\mathcal{B}$.

Given a circuit $\mathcal{C} = (x_1, ..., x_l)$, i.e. an ordered sequence of sites in Λ such that $(x_i, x_{i+1}) \in \mathcal{B}$ for $i = 1, 2, ..., l$, $x_{l+1} = x_1$, we define the magnetic flux $\Phi_{\mathcal{C}}$ through the circuit as

$$\Phi_{\mathcal{C}} = \sum_{i=1}^{n} \theta_{x_i x_{i+1}}, \qquad \mod 2\pi \tag{2.2}$$

For a (two-dimensional) planar lattice, given a set of magnetic fluxes through all faces, one can always find corresponding phases. These are uniquely determined up to a gauge

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* i.e. one can forget that the lattice is embedded in $\mathbf{R}^d$ and view $(\Lambda, \mathcal{B})$ as an abstract graph.

transformation, i.e. a unitary transformation with matrix elements $\mathcal{U}_{xy} = e^{i\phi_x} \delta_{xy}$ where ϕ_x is a real function on Λ, which gives $\theta_{xy} \to \theta'_{xy} = \theta_{xy} + (\phi_x - \phi_y)$. This gauge transformation leaves the spectrum of T unchanged. In higher dimensions given a set of magnetic fluxes across all faces it is not always possible to find phases θ_{xy} satisfying (2.2) (see [58] for more details).

We will be particularly concerned with bipartite lattices. These are the union of two disjoint sublattices, $\Lambda = A \cup B$, such that the edges of $\mathcal{B}$ never connect two sites of the same sublattice. In particular the matrix elements of T are non zero only if x and y are not on the same sublattice and the elements of T^2 connect only A to A or B to B. On such lattices T is unitarily equivalent to $-T$, the unitary transformation being $\epsilon_x \delta_{xy}$, $\epsilon_x = +1$ or -1, according to $x \in A$ or B. Thus the spectrum of T is a symmetric set about the origin (the set may contain zero).

With each site x in Λ is associated a random variable s_x with values $+1$ or -1. If $s_x = +1$, one can think of x as being occupied by a classical particle (ion, impurity, spin, localized f electron) and, if $s_x = -1$ as x being empty. With each ion configuration $\mathbf{s} = \{s_x\}$ on Λ, we associate the diagonal matrix S with elements $s_x \delta_{xy}$. Note that S is left unchanged by the unitary transformation $\epsilon_x \delta_{xy}$ as well as by any gauge transformation. In the following $N_i = N_i(\mathbf{s})$ denotes the number of ions in the configuration $\mathbf{s}$, i.e.

$$N_i = N_i(\mathbf{s}) = \frac{1}{2} \sum_{x \in \Lambda} (s_x + 1) \tag{2.3}$$

The hamiltonian for one quantum particle in a specified ion configuration $\mathbf{s}$ (or external potential) is

$$h_\Lambda(\mathbf{s}) = -T + US \tag{2.4}$$

where the coupling constant U is a given real number. If $U > 0$ the potential is repulsive and if $U < 0$ it is attractive. In (2.4) $h_\Lambda(\mathbf{s})$ is a $|\Lambda| \times |\Lambda|$ matrix acting on the one-particle Hilbert space $l^2(\Lambda)$ of wavefunctions $(\psi_x, x \in \Lambda)$ with $\sum_{x \in \Lambda} |\psi_x|^2 < \infty$. It has $|\Lambda|$ eigenvalues $e_1(\mathbf{s}) \le e_2(\mathbf{s}) \le ... \le e_{|\Lambda|}(\mathbf{s})$ with the following useful properties.

Structure of the spectrum: Let $max|t_{xy}| = t$ and $|U| > zt$, where z is the maximal coordination number of the lattice. Under these conditions, we have :

a) $e_i(\mathbf{s}) \in [-|U| - zt, -|U| + zt] \cup [|U| - zt, |U| + zt]$, $i = 1, ..., |\Lambda|$. Thus the spectrum consists of two "bands", one on the negative axis and one on the positive axis, and has a gap of width at least $2(|U| - zt)$.

b) For $U > zt$ (resp. $U < -zt$) the number of negative eigenvalues is equal to $|\Lambda| - N_i$ (resp N_i).

Here we have used the word "band" for convenience although the spectrum is discrete on a finite lattice. For periodic $\mathbf{s}$ on an infinitely large periodic lattice, this spectrum goes over to a continuous one consisting of several bands. Lattices of particular interest are the d-dimensional cubic ones which are bipartite and for which $z = 2d$, with or without periodic boundary conditions for t_{xy}. On such lattices if $\mathbf{s}$ is one of the chessboard configurations (i.e. $s_x = \epsilon_x$ or $s_x = -\epsilon_x$) the spectrum consists of two continuous bands.

The associated second quantized hamiltonian for spinless fermions (conduction electrons) is the Falicov-Kimball hamiltonian

$$H_\Lambda(\mathbf{s}) = - \sum_{x,y \in \Lambda} t_{xy} a_x^\dagger a_y + U \sum_{x \in \Lambda} s_x (a_x^\dagger a_x - \frac{1}{2}) \qquad (2.5)$$

where $a_x^\dagger$ and a_y, the creation and annihilation operators of a fermion at sites x and y, satisfy the usual anticommutation relations. This is a $2^{|\Lambda|} \times 2^{|\Lambda|}$ matrix acting on the Fock space of totally antisymmetric wave functions $(\oplus_0^{|\Lambda|} l^2(\Lambda^N))_-$. Strictly speaking the second quantization of (2.4) is (2.5) with $a_x^\dagger a_x$ instead of $(a_x^\dagger a_x - \frac{1}{2})$, however it turns out that the definition (2.5) is more convenient in the present setting, and amounts to redefine the chemical potential of the ions. Let us remark that the potential energy in (2.5) is

$$2U \sum_{x \in \Lambda} (n_x^{ion} - \frac{1}{2})(a_x^\dagger a_x - \frac{1}{2}) \qquad (2.6)$$

which is the convenient form to exploit particle-hole symmetry. For a specified configuration $\mathbf{s}$ (2.5) is the hamiltonian of a free Fermi gas in the external potential $U s_x$. However this is not true if we consider $\mathbf{s}$ to be a random variable, whose mean value will be such as to minimize the free energy. This induces an effective interaction between the electrons which makes the problem highly non trivial. Alternatively one can also consider that the electrons induce an effective interaction between the classical spins. The nature of this interaction and many of its properties will be elucidated.

We will also consider models where the spinless fermions are replaced either by hard-core bosons or by interacting spin one-half fermions. In the first case this amounts to replace $a_x^\dagger$, a_y in (2.5) by $b_x^\dagger$, b_y where the b's satisfy anticommutation relations if they are on the same site and commute if they are on different sites (see sect. 5). We remark that this algebra introduces an interaction between the bosons, which is very different from the Pauli principle. Indeed one can view this system as the limit of usual Bose particles with an infinite on-site repulsion. For the interacting spin one-half fermions (one can also take "spin one-half bosons", i.e. two independent species of hard-core bosons) a typical hamiltonian will contain a Hubbard interaction

$$
\begin{aligned}
H_\Lambda(\mathbf{s}) = -\sum_{x,y\in\Lambda,\sigma=\uparrow,\downarrow} t_{xy} a_{x\sigma}^\dagger a_{y\sigma} + U\sum_{x\in\Lambda,\sigma=\uparrow,\downarrow} s_x(a_{x\sigma}^\dagger a_{x\sigma} - \frac{1}{2}) \\
+ U'\sum_{x\in\Lambda}(a_{x\uparrow}^\dagger a_{x\uparrow} - \frac{1}{2})(a_{x\downarrow}^\dagger a_{x\downarrow} - \frac{1}{2})
\end{aligned}
\tag{2.7}
$$

However the results for the interacting cases are much more restricted and we will deal with them in section 5. The rest of this section concerns mainly the hamiltonian (2.5).

2.1. Ground State Energy and Gap

Canonical ensemble

For the FK hamiltonian (2.5) the ground state energy of N electrons in the configuration $\mathbf{s}$ is given by the sum of the lowest N eigenvalues

$$
E_N(\mathbf{s}) = \sum_{j=1}^{N} e_j(\mathbf{s}) - \frac{U}{2}\sum_{x\in\Lambda} s_x
\tag{2.8}
$$

A general expression valid also for the interacting bosonic or electronic models is $E_N(\mathbf{s}) = inf spec(H_\Lambda^N(\mathbf{s}))$ where $H_\Lambda^N(\mathbf{s})$ is the relevant hamiltonian (for example (2.7)) restricted to the N particle sector. We define the ground state energy for N electrons and N_i ions as

$$
E_{N,N_i} = min_{\mathbf{s},N_i(\mathbf{s})=N_i} E_N(\mathbf{s})
\tag{2.9}
$$

and the absolute ground state energy

$$
E_0 = min_{N,\mathbf{s}} E_N(\mathbf{s})
\tag{2.10}
$$

One of the main problems addressed in the next sections is to analyse the nature of minimizers s_0 in (2.9) and (N_0, s_0) in (2.10). For $U < 0$, the case $N_i = N$ is of particular importance since it corresponds to a "neutral" situation in the electron/ion interpretation [14]. On the other hand for $U > 0$ the case $N_i + N = |\Lambda|$ is important since it corresponds to the half filled band in the purely electronic interpretation [8].

Another quantity of interest is the "charge gap" defined as

$$G_{N,N_i} = \mu_+ - \mu_- \qquad (2.11)$$

where $\mu_+ = E_{N+1,N_i} - E_{N,N_i}$ and $\mu_- = E_{N,N_i} - E_{N-1,N_i}$ are respectively the energy variations when we add and remove one electron without changing the number of ions. $G_{N,N_i} > \epsilon$ means that a finite energy is needed to create an excitation corresponding to an infinitely separated electron-hole pair when there are N_i ions. Therefore it is reasonable to expect that the system is an insulator if there is a finite charge gap*. We make the trivial remark that even in the non-interacting case $G_{N,N_i} \neq e_{N+1}(s_0) - e_N(s_0)$, where s_0 is the minimizer of $E_{N,N_i}(s)$ in (2.9), because s_0 can be modified when we add or remove a particle. Therefore the proof of the existence of a charge gap is not a one body problem (even if s_0 is known) and this makes it non trivial.

In the rest of this paragraph we collect some useful formulas for (2.8) and (2.9). The discussion is valid for any dimension and lattice Λ, unless explicitely mentionned. Obviously we always have the lower bound

$$E_N(s) \geq \sum_{e_j < 0} e_j(s) - \frac{U}{2} \sum_{x \in \Lambda} s_x \qquad (2.12)$$

Moreover

$$\sum_{e_j < 0} e_j(s) = -\frac{1}{2}\left(\sum_{e_j < 0} |e_j(s)| - \sum_{e_j < 0} e_j(s) \right)$$

$$= -\frac{1}{2}\left(tr|h_\Lambda(s)| - tr h_\Lambda(s) \right) = -\frac{1}{2} tr|h_\Lambda(s)| + \frac{U}{2} \sum_{x \in \Lambda} s_x$$

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* We are not aware of any precise relationship between this notion of an insulator and transport properties.

and therefore [14,15]

$$E_N(\mathbf{s}) \geq -\frac{1}{2} tr|h_\Lambda(\mathbf{s})| \tag{2.13}$$

In (2.13) the absolute value of the hamiltonian means $\sqrt{h_\Lambda(\mathbf{s})^2}$.

If $max|t_{xy}| = t$, and $U < -zt$, by property (b), (2.12) and (2.13) become equalities for $N = N_i(\mathbf{s})$ (neutral situation). Therefore

$$
\begin{aligned}
E_{N=N_i(\mathbf{s})}(\mathbf{s}) &= -\frac{1}{2} tr \sqrt{T^2 + U^2 + U(TS + ST)} \\
&= -\frac{|U|}{2} tr \sqrt{I + U^{-1}(TS + ST) + U^{-2}T^2}
\end{aligned}
\tag{2.14}
$$

We can expand the square root in (2.14) to obtain the U^{-1} expansion of $E_{N=N_i(\mathbf{s})}(\mathbf{s})$ [37]. Another more systematic way to obtain the same expansion is to use the representation (by property (b) and (2.8))

$$E_{N=N_i(\mathbf{s})} = -\frac{U}{2} \sum_{x \in \Lambda} s_x + \int_C \frac{dz}{2\pi i} Tr \left[\frac{z}{z - h_\Lambda(\mathbf{s})} \right] \tag{2.15}$$

where C is a contour in the complex plane enclosing all the negative eigenvalues, and to iterate the resolvent identity

$$\frac{1}{z - h_\Lambda(\mathbf{s})} = \frac{1}{z - US} - \frac{1}{z - US} T \frac{1}{z - h_\Lambda(\mathbf{s})} \tag{2.16}$$

which yields

$$
\begin{aligned}
E_{N=N_i(\mathbf{s})}(\mathbf{s}) &= -\frac{U}{2} \sum_{x \in \Lambda} s_x + \sum_{k \geq 0} (-1)^k \int_C \frac{dz}{2\pi i} Tr \left(\left[\frac{1}{z - US} T \right]^k \frac{z}{z - US} \right) \\
&= \frac{U}{2}|\Lambda| + \sum_{k \geq 2} (-1)^k \int_C \frac{dz}{2\pi i} Tr \left(\left[\frac{1}{z - US} T \right]^k \frac{z}{z - US} \right)
\end{aligned}
\tag{2.17}
$$

The contour integral in (2.17) equals

$$
\begin{aligned}
\sum_{x_1,\ldots,x_k} (-1)^k t_{x_1 x_2} t_{x_2 x_3} \ldots t_{x_k x_1} &\int_C \frac{dz}{2\pi i} \frac{z}{(z - U s_{x_1})^2} \prod_{j=2}^{k} \frac{1}{z - U s_{x_j}} \\
&= \frac{1}{(2U)^{k-1}} \sum_{x_1,\ldots,x_k}' t_{x_1 x_2} t_{x_2 x_3} \ldots t_{x_k x_1} \\
&\quad \times (-1)^{p-1} \frac{(k-2)!}{(p-1)!(k-p)!} \frac{k+1-2p}{2}
\end{aligned}
\tag{2.18}
$$

where $\sum'$ means that $(x_1, ..., x_k)$ contains at least one empty site and one occupied site and p is the number of x_j with $s_{x_j} = -1$ in $(x_1, ..., x_k, x_1)$. Introducing m, the number of x_j with $s_{x_j} = -1$ in $(x_1, ..., x_k)$ (i.e. the number of empty sites in $x_1, ..., x_k$) the formula (2.17) can be written as

$$
\begin{aligned}
E_{N=N_i(\mathbf{s})}(\mathbf{s}) = 2U \Bigg[\frac{1}{4}|\Lambda| - \sum_{k \geq 2} \frac{1}{(2U)^k} \sum_{x_1, ..., x_k}{}' (-1)^m t_{x_1 x_2} t_{x_2 x_3} ... t_{x_k x_1} \\
\times \frac{(k-2)!}{(m-1)!(k-m-1)!} \frac{1}{k} \Bigg]
\end{aligned}
\tag{2.19}
$$

and this expansion is convergent for $U < -zt$. We should also remark that the constraint on the sum over $X = (x_1, x_2, ..., x_k)$ and the factor $(-1)^m$ can be taken care of with the function

$$
\frac{1}{2^{k-1}} \left(2^{k-1} - 1 - \sum_{\emptyset \neq Y \subset X, |Y| even} S_Y \right) S_X, \qquad S_Y = \prod_{y \in Y} S_y
\tag{2.20}
$$

which leads to an explicit formula for the coefficients $K_X(U)$ in

$$
E_{N=N_i(\mathbf{s})}(\mathbf{s}) = \sum_{X \subset \Lambda} K_X(U) S_X
\tag{2.21}
$$

On a bipartite lattice the first sum in (2.19) is only over even values of k and thus the energy of the neutral ground state is invariant under a particle-hole transformation. The expansion (2.19) has been used by Lemberger [36] to study the ground state configuration in one dimension (see sect. 3). A similar expression can be given for $U > zt$ with $E_{N=|\Lambda|-N_i(\mathbf{s})}(\mathbf{s})$ replacing $E_{N=N_i(\mathbf{s})}(\mathbf{s})$.

Remark: one can show the convergence of the sum over k only for contours $\mathcal{C}$ enclosing all negative eigenvalues. In other words this method is not applicable in the non neutral (or non half-filled) situation.

Grand canonical ensemble

In the grand canonical ensemble we fix the chemical potentials (μ_e, μ_i) of the electrons and ions and minimize over all possible ion configurations $\mathbf{s}$ the function (from (2.5))

$$
E_\Lambda(\mathbf{s}, \mu_e, \mu_i) = \sum_{e_j(\mathbf{s}) \leq \mu_e} (e_j(\mathbf{s}) - \mu_e) - \frac{U}{2} \sum_{x \in \Lambda} s_x - \mu_i N_i(\mathbf{s})
\tag{2.22}
$$

By the same argument as in (2.13)

$$E_\Lambda(\mathbf{s}, \mu_e, \mu_i) = -\frac{1}{2}tr|h_\Lambda(\mathbf{s}) - \mu_e| - \mu_i N_i(\mathbf{s}) - \frac{\mu_e}{2}|\Lambda| \qquad (2.23)$$

Again one can derive the U^{-1} expansions in a similar way. Indeed if $U < -zt$ and if the chemical potential μ_e is in the gap (recall properties (a), (b)) the number of electrons is equal to N_i so that

$$E_\Lambda(\mathbf{s}, \mu_e, \mu_i) = E_{N=N_i(\mathbf{s})}(\mathbf{s}) - (\mu_i + \mu_e)N_i(\mathbf{s}) \qquad (2.24)$$

Thus the U^{-1} expansions in the canonical and grand canonical settings are equivalent. For $U > zt$, and μ_e in the gap, one has to replace the neutrality conditions $N = N_i(\mathbf{s})$ by the half-filling condition $N = |\Lambda| - N_i(\mathbf{s})$ and (2.24) becomes

$$E_\Lambda(\mathbf{s}, \mu_e, \mu_i) = E_{N=|\Lambda|-N_i(\mathbf{s})}(\mathbf{s}) - (\mu_i - \mu_e)N_i(\mathbf{s}) - \mu_e|\Lambda| \qquad (2.25)$$

For bipartite lattices the origin $(0,0)$ is an important point in the (μ_e, μ_i) plane. There (2.23) becomes $E_\Lambda(\mathbf{s}, 0, 0) = -\frac{1}{2}tr|h_\Lambda(\mathbf{s})|$ which is an even function of $\mathbf{s}$. In other words for $\mu_e = \mu_i = 0$ the energy is invariant under the particle-hole transformation for the ions $(\mathbf{s} \rightarrow -\mathbf{s})$. Indeed under the unitary transformation $\epsilon_x \delta_{xy}$, $h_\Lambda(\mathbf{s}) \rightarrow -h_\Lambda(-\mathbf{s})$. As we will see this property persists at finite temperatures.

The reader may wonder why we do not perform small U expansions. The reason is that an expansion of $[T^2 + U^2 + U(TS + ST)]^{1/2}$ involves $[T^2]^{-1/2}$ and since in general T has zero eigenvalues in the thermodynamic limit, the radius of convergence of the expansion goes to zero as the lattice size goes to infinity. For the moment there does not exist to our knowledge any analytical approach specific to small U, except for the one used in the one dimensional case ([46], sect. 3).

2.2. Finite Temperatures and Effective Interactions

The partition function at inverse temperature β and chemical potential μ_e, μ_i is

$$Z_\Lambda(\beta, \mu_e, \mu_i) = \sum_{\mathbf{s}} Tr \exp\left(-\beta(H_\Lambda(\mathbf{s}) - \mu_e N_e - \mu_i N_i(\mathbf{s}))\right) \qquad (2.26)$$

The sum is over all possible $2^{|\Lambda|}$ ions configurations and the trace is over the electronic Fock space.

Effective interaction between ions

The effective interaction F_Λ between ions, induced by the electrons, is defined by

$$e^{-\beta F_\Lambda(\mathbf{s},\beta,\mu_e,\mu_i)} = Tr \exp\left(-\beta(H_\Lambda(\mathbf{s}) - \mu_e N_e - \mu_i N_i(\mathbf{s}))\right) \qquad (2.27)$$

With this definition (2.26) becomes

$$Z_\Lambda(\beta,\mu_e,\mu_i) = \sum_{\mathbf{s}} e^{-\beta F_\Lambda(\mathbf{s},\beta,\mu_e,\mu_i)} \qquad (2.28)$$

which is the partition function of a classical spin system with a complicated temperature dependent interaction. It should be remarked that F_Λ is invariant under any gauge transformation. We can always write it as

$$F_\Lambda(\mathbf{s},\beta,\mu_e,\mu_i) = \sum_{X \subset \Lambda} J_X(\beta,\mu_e,\mu_i) \prod_{x \in X} s_x \qquad (2.29)$$

and the problem is to obtain some information over the potentials J_X. Then one may apply results and techniques of classical statistical mechanics. This approach is general and covers also the models with hard-core bosons and electron-electron interactions, but of course the practical computation of J_X is much more difficult.

For the FK hamiltonian (2.5), since the electrons do not interact (except for the Fermi statistics) for a given $\mathbf{s}$ we can perform exactly the trace in (2.27) and we get

$$F_\Lambda(\mathbf{s},\beta,\mu_e,\mu_i) = -\frac{1}{\beta} tr log(1 + e^{-\beta(h_\Lambda(\mathbf{s}) - \mu_e)}) - \frac{1}{2}(\mu_i + U)\sum_{x \in \Lambda} s_x - \frac{\mu_i}{2}|\Lambda| \qquad (2.30)$$

which can be rewritten as

$$F_\Lambda(\mathbf{s},\beta,\mu_e,\mu_i) = -\frac{1}{\beta} tr log cosh\left[\frac{\beta}{2}(h_\Lambda(\mathbf{s}) - \mu_e)\right] - \frac{1}{2}\mu_i \sum_{x \in \Lambda} s_x - \frac{1}{2}(\mu_e + \mu_i)|\Lambda| - \frac{|\Lambda|}{\beta} log 2 \qquad (2.31)$$

This formula is the generalisation of (2.23) to finite temperatures. Indeed *cosh* is an even function so we can replace $h_\Lambda(\mathbf{s}) - \mu_e$ by

$$|h_\Lambda(\mathbf{s}) - \mu_e| = \sqrt{(h_\Lambda(\mathbf{s}) - \mu_e)^2} \qquad (2.32)$$

This enables us to take the low temperature limit and to verify that $lim_{\beta \to \infty} F_\Lambda(\mathbf{s}, \beta, \mu_e, \mu_i)$ is equal to (2.23).

2.3. Symmetries

The hamiltonians (2.5) and (2.7) have symmetry properties which are related to the particle-hole transformations for ions and for electrons. Writing explicitely the U dependence we have

$$H_\Lambda(\mathbf{s}, U) = H_\Lambda(-\mathbf{s}, -U) \qquad N_i(\mathbf{s}) = |\Lambda| - N_i(-\mathbf{s}) \tag{2.33}$$

and thus

$$E_N(\mathbf{s}, U) = E_N(-\mathbf{s}, -U) \tag{2.34}$$

$$E_\Lambda(\mathbf{s}, \mu_e, \mu_i, U) = E_\Lambda(-\mathbf{s}, \mu_e, -\mu_i, -U) - \mu_i|\Lambda| \tag{2.35}$$

$$F_\Lambda(\mathbf{s}, \beta, \mu_e, \mu_i, U) = F_\Lambda(-\mathbf{s}, \beta, \mu_e, -\mu_i, -U) - \mu_i|\Lambda| \tag{2.36}$$

which shows that we can restrict the discussion to $U > 0$ (or $U < 0$).

Discrete Symmetries on a Bipartite Lattice

We discuss the spin flip, electron-hole, and time reversal, transformations on bipartite lattices $\Lambda = A \cup B$. The spin flip (or particle-hole transformation for ions) F is defined by $FSF = -S$. The electron-hole transformation W is unitary, with $W^\dagger = W$, and

$$W a_x^\dagger W = \epsilon_x a_x, \qquad W a_x W = \epsilon_x a_x^\dagger \tag{2.37}$$

with $\epsilon_x = 1$ for bosons, and $\epsilon_x = 1$, $x \in A$, $\epsilon_x = -1$, $x \in B$ for fermions. The time reversal transformation is an antilinear operator J. For any matrix A, $JAJ = A^*$ where A^* is obtained by replacing the elements of A by their complex conjugate. So J^2 is the identity and for any operator A, $Tr(JAJ) = (TrA)^*$. In particular since the creation and annihilation operators have real matrix representations, for any complex number α

$$J(\alpha a_x^\dagger)J = \alpha^* a_x^\dagger, \qquad J(\alpha a_x)J = \alpha^* a_x \tag{2.38}$$

We then have $FH_\Lambda(\mathbf{s})F = H_\Lambda(-\mathbf{s})$, $WH_\Lambda(\mathbf{s})W = H_\Lambda(-\mathbf{s})^*$, $JH_\Lambda(\mathbf{s})J = H_\Lambda(\mathbf{s})^*$ and

$$JW[H_\Lambda(\mathbf{s}) - \mu_e N - \mu_i N_i(\mathbf{s})]WJ = H_\Lambda(-\mathbf{s}) + \mu_e N + \mu_i N_i(-\mathbf{s}) - (\mu_e + \mu_i)|\Lambda| \tag{2.39}$$

which implies

$$E_N(\mathbf{s}) = E_{|\Lambda|-N}(-\mathbf{s}) \tag{2.40}$$

$$E_\Lambda(\mathbf{s}, \mu_e, \mu_i) = E_\Lambda(-\mathbf{s}, -\mu_e, -\mu_i) - (\mu_e + \mu_i)|\Lambda| \tag{2.41}$$

$$F_\Lambda(\mathbf{s}, \beta, \mu_e, \mu_i) = F_\Lambda(-\mathbf{s}, \beta, -\mu_e, -\mu_i) - (\mu_e + \mu_i)|\Lambda| \tag{2.42}$$

These relations show that the origin of the chemical potential plane, $(\mu_e, \mu_i) = (0, 0)$ is the symmetry point of the system

$$F_\Lambda(\mathbf{s}, \beta, 0, 0) = F_\Lambda(-\mathbf{s}, \beta, 0, 0) \tag{2.43}$$

$$E_\Lambda(\mathbf{s}, 0, 0) = E_\Lambda(-\mathbf{s}, 0, 0) \tag{2.44}$$

i.e. the effective interaction and the (grand canonical) energy, are invariant under the particle hole transformation for ions.

Combining (2.35-2.36) and (2.41-2.42) we obtain

$$F_\Lambda(\mathbf{s}, \beta, \mu_e, \mu_i, U) = F_\Lambda(\mathbf{s}, \beta, -\mu_e, \mu_i, -U) - \mu_e|\Lambda| \tag{2.45}$$

$$E_\Lambda(\mathbf{s}, \beta, \mu_e, \mu_i, U) = E_\Lambda(\mathbf{s}, \beta, -\mu_e, \mu_i, -U) - \mu_e|\Lambda| \tag{2.46}$$

i.e. the origin of the chemical potential plane is also the symmetry point with respect to the transformation $U \to -U$.

Finaly we remark that

$$FJW[H_\Lambda(\mathbf{s}) - \mu_e N - \mu_i N_i(\mathbf{s})]WJF = H_\Lambda(\mathbf{s}) + \mu_e N + \mu_i N_i(\mathbf{s}) - (\mu_e + \mu_i)|\Lambda| \tag{2.47}$$

and thus at the symmetry point $\mu_e = \mu_i = 0$ on a bipartite lattice the hamiltonian $H_\Lambda(\mathbf{s})$ (2.5) or (2.7) is invariant under FJW.

Continuous symmetries

The hamiltonians (2.5), (2.7) commute with the total electron number $N = \sum_{x \in \Lambda} a_x^\dagger a_x$ or $N = \sum_{x \in \Lambda, \sigma=\uparrow,\downarrow} a_{x\sigma}^\dagger a_{x\sigma}$. They are thus invariant under the $U(1)$ transformation

$$a_x \to e^{i\theta N} a_x e^{-i\theta N} \tag{2.48}$$

One can show that the $U(1)$ symmetry is not broken in one and two dimensions, using a method devised by McBryan and Spencer [59] for classical systems, and adapted to the quantum case [60], [61]. We denote by $< - >$ the average in the thermodynamic limit for fixed (β, μ_e, μ_i). The following results have been proved [61] for $\Lambda \subset \mathbf{Z}^d$ and $t_{xy} \neq 0$ even if x and y are not nearest neighbours:

a) $d = 1$: if $|t_{xy}|$ decays faster than $|x - y|^{-\alpha}$, $\alpha > 2$, then $< a_{x\sigma}^{\dagger} a_{y\sigma} >$ tends to zero faster than $|x - y|^{-(\alpha-1)}$ and thus there is no off-diagonal long range order. Also $< a_{x\uparrow}^{\dagger} a_{x\downarrow}^{\dagger} a_{y\downarrow} a_{y\uparrow} >$ tends to zero like $|x - y|^{-2(\alpha-1)}$ and there is no superconducting long range order. Moreover, if t_{xy} decays exponentially then these correlations also do. These results remain valid in the zero temperature limit.

b) $d = 2$: if $\alpha > 4$, then both type of correlations decay algebraically (even if the hopping decays exponentially) with a power depending on the temperature. The power tends to zero as β^{-1}, for $\beta \to \infty$, and thus we do not have information for the ground state.

These results, and the same proofs, extend also to hard-core bosonic systems.

The hamiltonian (2.7) also conserves the electronic spin. The same methods, and also older ones [62], [63], give similar results concerning the absence of magnetic long range order. We refer the reader to the literature.

2.4. Observables

The average value of an observable $O(\{a_x^{\dagger}, a_x, s_x\})$ is

$$< O(\{a_x^{\dagger}, a_x, s_x\}) >_\Lambda (\beta, \mu_e, \mu_i) = \frac{1}{Z_\Lambda} \sum_{\mathbf{s}} Tr O(\{a_x^{\dagger}, a_x, s_x\})$$
$$\times \exp(-\beta(H_\Lambda(\mathbf{s}) - \mu_e N_e - \mu_i N_i(\mathbf{s}))) \quad (2.49)$$

If the observable does not depend on $a_x^{\dagger}$, a_x we can again integrate the electrons and the average reduces to

$$< O(s_x) >_\Lambda (\beta, \mu_e, \mu_i) = \frac{1}{Z_\Lambda} \sum_{\mathbf{s}} Tr O(s_x) \exp(-\beta F_\Lambda(\mathbf{s}, \beta, \mu_e, \mu_i)) \quad (2.50)$$

When boundary conditions are not specified, like in (2.50), (2.51), it is understood that we have free boundary conditions. On a bipartite lattice, the averages at the symmetry

point $(\mu_e = 0, \mu_i = 0)$ will be denoted by $< - >_\Lambda (\beta)$. In particular for free boundary conditions, on any finite bipartite lattice

$$< a_x^\dagger a_x >_\Lambda (\beta) = \frac{1}{2}, \qquad \text{all} \qquad x \in \Lambda \tag{2.51}$$

$$< a_x^\dagger a_y >_\Lambda (\beta) = 0, \qquad x \neq y \qquad \text{if} \qquad x, y \in A \qquad \text{or} \qquad x, y \in B \tag{2.52}$$

$$< s_x >_\Lambda (\beta) = 0, \qquad \text{all} \qquad x \in \Lambda \tag{2.53}$$

Proof of (2.51) - (2.53) : It uses the electron-hole symmetry and the time reversal operator, discussed in section 2.3. Let $Y = JFW$ be the combination of the electron-hole W, spin flip F, and time reversal J transformations. We have $Y^2 = I$ (the identity) and $Tr(YOY) = (TrO)^*$ because J is antilinear. On a bipartite lattice $H_\Lambda(\mathbf{s})$ is invariant under Y, thus

$$
\begin{aligned}
Tr a_x^\dagger a_y e^{\beta H_\Lambda(\mathbf{s})} &= \left(TrY a_x^\dagger Y^2 a_y Y^2 e^{-\beta H_\Lambda(\mathbf{s})} Y \right)^* \\
&= \epsilon_x \epsilon_y \left(Tr a_x a_y^\dagger e^{-\beta H_\Lambda(\mathbf{s})} \right)^* \\
&= \epsilon_x \epsilon_y Tr(\delta_{xy} - a_x^\dagger a_y) e^{-\beta H_\Lambda(\mathbf{s})}
\end{aligned}
\tag{2.54}
$$

In the last equality the cyclicity of the trace and the anticommutation relation for fermions were used. Finaly (2.54) is equivalent to (2.51), (2.52). For (2.53) we use that $< s_x >_\Lambda (\beta)$ is real and $Y s_x Y = -s_x$.

Remarks :

a) In the case of hard-core bosons a similar discussion yields (2.51) and (2.53) (but not (2.52)).

b) These formulas are valid for any finite bipartite lattice and thus there is no finite size effect on these correlation functions at the symmetry point. Moreover the amplitude of the hopping can be arbitrary and one can replace the coupling constant U of the on site interaction by local ones U_x. They are valid for a more general class of hamiltonians than (2.5) or (2.7). However they are not true if we break the symmetry by an external field or special boundary conditions. We refer to [64] for a detailled discussion.

We mention without proof the following formula [65] which holds for the hamiltonian (2.5) on a bipartite lattice and for any boundary condition (so that (2.51)-(2.53) are not

necessarily satisfied),

$$< a_x^\dagger a_x >_\Lambda^{b.c} (\beta) = \frac{1}{2} - g(\beta, U) < s_x >_\Lambda^{b.c} (\beta) \tag{2.55}$$

with

$$g(\beta, U) = tr \left(\frac{1}{\sqrt{T^2 + U^2}} tanh \left[\frac{\beta}{2} \sqrt{T^2 + U^2} \right] \right) \tag{2.56}$$

This formula shows in particular that the critical behaviour of the average electronic density is the same than that of the spins.

3. ONE DIMENSION : GROUND STATES

A large number of investigations [13,35–52] have been devoted to the study of the ground states of the one dimensional Falicov-Kimball model with nearest neighbour interactions ($t_{xy} = t$ if $|x - y| = 1$ and zero otherwise), using either the canonical or the grand canonical formalism. To be specific we restrict the discussion to the attractive case $U < 0$ and define the electron and ion densities as $\rho_e = \frac{N}{|\Lambda|}$ and $\rho_i = \frac{N_i}{|\Lambda|}$.

Following [36,39] we introduce the definition:

for $\rho_e = \frac{p}{q}$ with p relatively prime to q and $\rho_i = \frac{p'}{q}$ (p' not necessarily prime relative to q), the *"most homogeneous configuration of ions"* is the periodic configuration with period q where the positions $\{k_j\}$ of the ions in the cell $[0, 1, ..., q - 1]$ are given by the solutions of

$$pk_j = j \qquad \mod q, \qquad j = 0, 1, ..., p' - 1 \tag{3.1}$$

3.1 Canonical Ensemble

On the basis of numerical evidence, Freericks and Falicov [39] formulated the following two conjectures:

1) For *neutral systems* ($\rho_e = \rho_i$) the ground state is realised by the most homogeneous configuration of ions (3.1).

2) For *non-neutral systems* ($\rho_e \neq \rho_i$), there exist an increasing function $0 \leq b(|U|) < 1$ with $b(0) = 0$, $b(\infty) = 1$, such that for $\rho_e < b(|U|)\rho_i < \rho_i$ the ground state is realised by the *"segregated configuration"*, where all ions clump together. This ground state can be

understood as a mixture of the vacuum ($\rho_e = \rho_i = 0$) and the full configuration ($\rho_i = 1$, $\rho_e \neq 0$). Similarly for $\rho_e > 1 - b(|U|)\rho_i > 1 - \rho_i$, the ground state is the segregated configuration, mixture of ($\rho_e = \rho_i = 1$) and the empty configuration ($\rho_i = 0, \rho_e \neq 0$).

Then, using formal second order Rayleigh-Schrödinger perturbation theory they arrived at the following third conjecture [39]:

3) In the limit $U \to 0$ and for ($\rho_e = \frac{p}{q}, \rho_i = \frac{p'}{q}$), with p relatively prime to q, the ground state is realised by the most homogeneous configuration (3.1).

For large $|U|$ the first two conjectures were proven by Lemberger [36]. In the neutral case, for any rational density $\rho_e = \rho_i = \frac{p}{q}$, there exists a function $U_c^{hom}(q)$ such that for $|U| > U_c^{hom}(q)$ the ground state is the most homogeneous configuration of ions (3.1). His estimates give $U_c^{hom}(q) \sim a^q$ with some numerical constant a. However the proof does not give any indication about the optimal value of U_c^{hom}, in particular whether it might be independent of q. On the other hand, for the special value $\rho_e = \rho_i = 1/2$ it is known that $U_c^{hom} = 0$ [14]. Thus following [39] it was conjectured that $U_c^{hom} = 0$ for all densities, but as we shall see this cannot be true for densities close to zero or one.

A qualitative explanation of this property was given in [52]. It was shown that for large U, and to leading order in U^{-1}, the energy of the neutral system is given by a two body potential of the form $2(d+1)\exp(-\lambda(2d+1))$, where d is the distance between two ions, and $\lambda = |\ln\frac{1}{2}[(U^2+4)^{1/2} - U]|$. In other words, for large U, an equal number of electrons and ions will form neutral atoms which repel each other with an effective two body potential, which is convex and decreasing. Using the result of Hubbard [66], it then follows that the most homogeneous configuration yields indeed the minimum energy. With this analysis it is again not possible to decide whether U_c^{hom} is independent of q.

For the non neutral case $\rho_e \neq \rho_i$, Lemberger [36] was able to prove the second conjecture for large U: if $U > U_c^{seg}(\rho_e/\rho_i)$ then the ground state is the segregated configuration. (See also [41,43,49]).

To investigate the validity of the conjecture in the small U limit a systematic numerical analysis was initiated in [42] (see also [45] where canonical phase diagrams are obtained by translating results from the grand canonical ensemble). For a large number of periodic and

aperiodic configurations the energy was obtained by means of exact numerical calculations and compared to find the configuration with minimum energy.

Looking at finite (512 sites) as well as infinite systems, it was established that the first conjecture could not be correct for small $|U|$: for neutral systems with $\rho_e = \rho_i = \rho = p/q < 1/4$ there exist periodic configurations, with period larger than q, and energy smaller than the energy of the most homogeneous configurations. Furthermore, it was observed that there exists a function $U_c(\rho)$ which is, decreasing from $\frac{t}{\sqrt{3}}$ to 0 for $\rho \in [0, \frac{1}{4}]$, vanishing for $\rho \in [\frac{1}{4}, \frac{3}{4}]$, increasing from 0 to $\frac{t}{\sqrt{3}}$ for $\rho \in [\frac{3}{4}, 1]$, with the following critical property. For $|U| > U_c(\rho)$ the ground state is the most homogeneous configuration, while for $|U| < U_c(\rho)$ the ground state is a mixture of some periodic configuration (3.1) with the empty configuration ($\rho_i = 0, \rho_e \neq 0$) if $\rho_i < 1/4$, or with the full configuration ($\rho_i = 1, \rho_e \neq 0$) if $\rho_i > 3/4$. In other words there is phase separation. To see what kind of periodic configurations appear for $|U| < U_c(\rho)$ all mixtures consisting of the empty configuration with some periodic configuration of period $q \leq 10$ were considered for $\rho = 1/5, 1/6, 1/7, 1/10$. In this analysis the only periodic configuration which appeared were made of equally spaced p-molecules (i.e. p consecutive sites occupied by ions followed by $q - p$ empty sites), with one electron per molecule.

These results were recently confirmed by an analytical calculation valid for $U \to 0$ [46]. The Rayleigh-Schrödinger perturbation theory used in [39] contains, already at second order small denominators which vanish for some values of the density, and thus is not reliable. The correct approach is to use nearly degenerate perturbation theory (as in band theory [67]). Then the ground state energy of a periodic configuration is of the form

$$E(\rho_e, \mathbf{s}) = -\frac{2t}{\pi} \sin 2\pi \rho_e - U\rho_e\rho_i + \frac{1}{4\pi t} \frac{|W(2\pi\rho_e, \mathbf{s})|^2}{\sin 2\pi \rho_e} U^2 \ln U + O(U^2) \qquad (3.2)$$

where $|W|^2$ is the structure factor of the configuration $\mathbf{s}$ evaluated at the wave vector $2\pi\rho_e$. This formula is presumably rigorously true if $Uq << 1$ although in [46] it is not proven that the remainder is indeed $O(U^2)$ for a given q and uniformly with respect to $\mathbf{s}$. The $U^2 \ln U$ term (which is reminiscent of the theory of the Peierls instability [68]) is much bigger than $O(U^2)$ and therefore the properties of the ground state are found by analysing the structure factor.

Let us describe the result obtained in [46]. Let $\rho_c \simeq 0,3710$ be the solution of $2\pi\rho_c = \tan\pi\rho_c$. Given the integer q, let $\tilde{p}/q$ be the largest rational in the set $R_q = \{p'/q; p' = 0, 1, ..., q\}$ which is smaller than ρ_c, and $\bar{p}/q$ the smallest rational in R_q larger than $(1-\rho_c)$. We then introduce

$$\frac{p'}{q} = \begin{cases} \frac{\tilde{p}}{q} < \rho_c & \text{if } \tilde{p} \text{ satisfies (3.5) below} \\ \frac{(\tilde{p}+1)}{q} > \rho_c & \text{otherwise} \end{cases} \tag{3.3}$$

$$\frac{p''}{q} = \begin{cases} \frac{\bar{p}}{q} > 1 - \rho_c & \text{if } \bar{p} \text{ satisfies (3.6) below} \\ \frac{(\bar{p}-1)}{q} < 1 - \rho_c & \text{otherwise} \end{cases} \tag{3.4}$$

with

$$\sin\pi\frac{\tilde{p}}{q} > \left(\frac{\tilde{p}}{\tilde{p}+1}\right)^{1/2} \sin\pi\frac{\tilde{p}+1}{q} \tag{3.5}$$

$$\sin\pi\frac{\bar{p}}{q} > \left(\frac{q-\bar{p}}{q-\bar{p}+1}\right)^{1/2} \sin\pi\frac{\bar{p}-1}{q} \tag{3.6}$$

Property:

Let $\rho_e = p/q$ with p relatively prime to q, and p', p'' be given by (3.3), (3.4).

a) If $\rho_i = p_i/q$ with $p_i \in \{p', p'+1, ..., p''\}$ then for $|U|$ sufficiently small the ground state is the most homogeneous configuration (3.1). In particular this is the case for $\rho_i = p_i/q$ with $\rho_i \in [\rho_c, 1-\rho_c]$, and thus also for neutral systems with $\rho_e = \rho_i \in [\rho_c, 1-\rho_c]$.

b) For all other rational ion densities ρ_i, and $|U|$ sufficiently small, the ground state is a mixture of two most homogeneous configurations (3.1) with ion densities:

$$0 \text{ and } p'/q \text{ if } \rho_i \in]0, \tfrac{p'}{q}[,$$

$$p_i/q \text{ and } (p_i+1)/q \text{ if } \rho_i \in]\tfrac{p'}{q}, \tfrac{p''}{q}[,$$

$$p''/q \text{ and } 1 \text{ if } \rho_i \in]\tfrac{p''}{q}, 1[.$$

In particular for $\rho_i < 1/4$ and $\rho_i > 3/4$ the ground state is always a mixture (in the limit $|U| \to 0$) and thus for neutral systems with density smaller than 1/4 or greater than 3/4, the ground state is also a mixture.

This property shows that the periodicity of the pure phase is given by the denominator of the electron density: it is the smallest period necessary to open a gap at the Fermi level. It also follows from (3.2) that to leading order in U the electron density is uniform even when the state is a mixture.

For $\rho_i < p'/q$ and $\rho_i > p''/q$ the phase separated state is a mixture of a metallic state (empty or full lattice) and an insulating state (period q phase). If $\rho_e = \rho_i = \rho$ and $\rho \in [\rho_c, 1 - \rho_c]$, or $\rho = p'/q$, or $\rho = p''/q$, the ground state is the same as the one found by Lemberger for large $|U|$. It is therefore reasonable to expect that for these densities the ground state does not have any phase transition when $|U|$ is increased from 0 to ∞. This seems to be confirmed for intermediate values of U by the numerical simulations. Moreover there will be a phase transition as $|U|$ varies for $\rho \in [0, \rho_c]$ or $[1 - \rho_c, 1]$ $\rho \neq \tilde{p}/q$, $\bar{p}/q$

3.2 Grand Canonical Ensemble

To extend these investigations to arbitrary values of U and densities, and to avoid the difficulties associated with mixtures, it is more convenient to work in the grand canonical formalism (sect. 2.1). This was done in [40,42] by means of exact numerical calculations. Phase diagrams* in the chemical potential plane are represented in figure 1 for the case $|U| > 2t$ and in figure 2 for $|U| < 2t$.
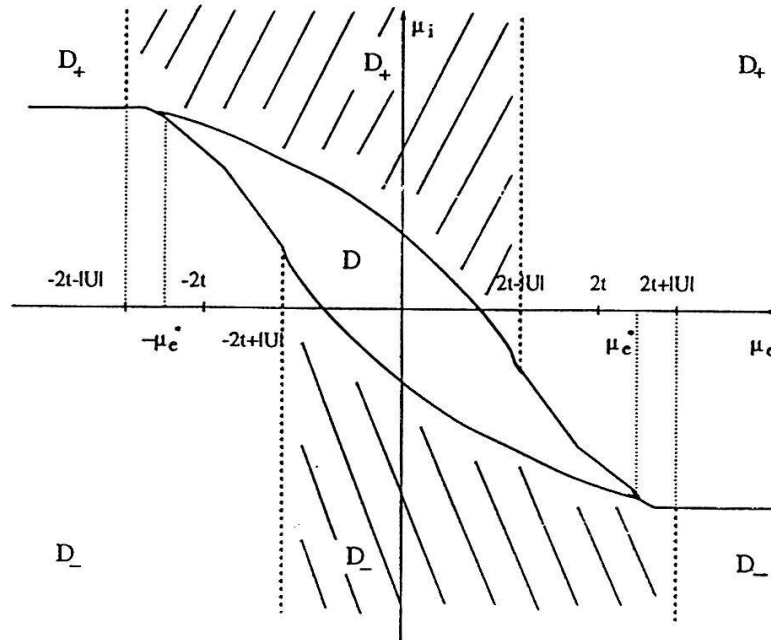

Figure 1a: Phase diagram of the one dimensional FK model, for $-2t < U < 0$, in the (μ_e, μ_i) plane.

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* These phase diagrams have not been established completely rigorously.
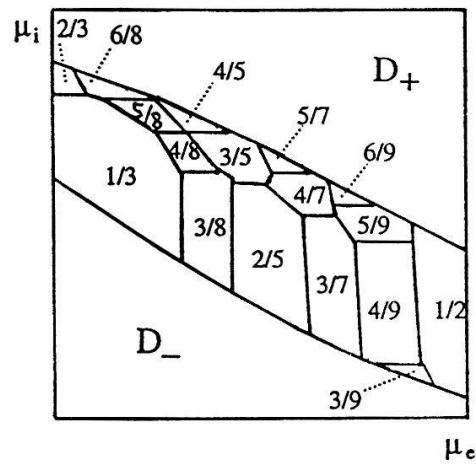
Figure 1b: A part of the domain D in fig.1a for $-2t < U < 0$ and $\mu_e < 0$(here $U = -0.3t$).
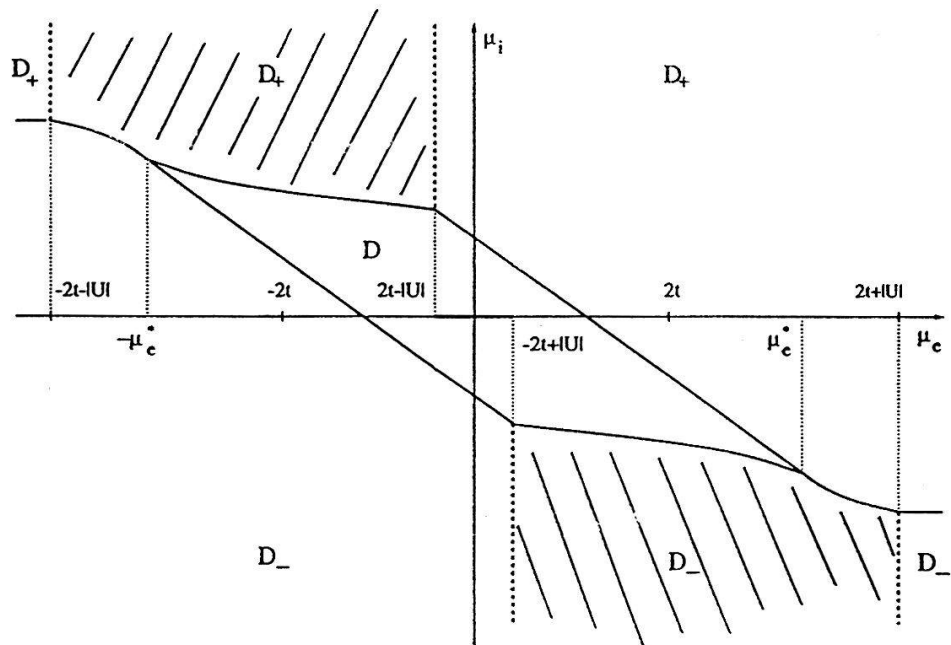

Figure 2a: Phase diagram of the one dimensional FK model, for $U < -2t$, in the (μ_e, μ_i) plane.
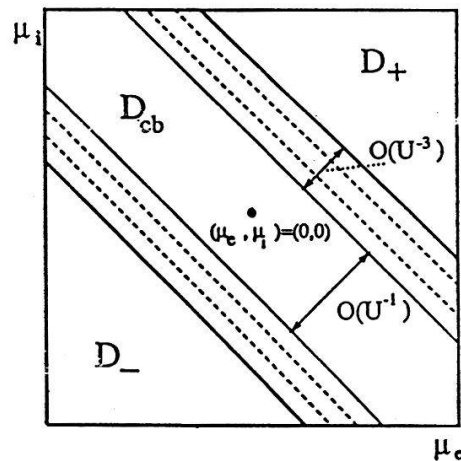
Figure 2b: A part of the domain D in fig 2a for $U < -2t$.
The origin of the (μ_e, μ_i) plane is at the center.

One observes the following structure (fig. 1a and 2a). The chemical potential plane (μ_e, μ_i) is decomposed into three connected parts D_-, D_+, and D. In the domain D_+ the ground state is the full configuration $(\rho_i = 1)$ with ρ_e increasing from 0 to 1 as μ_e increases from $-2t - |U|$ to $2t - |U|$; similarly in D_- the ground state is the empty configuration $(\rho_i = 0)$ with ρ_e increasing from 0 to 1 as μ_e increases from $-2t + |U|$ to $2t + |U|$. Furthermore there exists $\mu_e^* = \mu_e^*(U) > |2t - |U||$, such that D appears only in the strip $[-\mu_e^*, \mu_e^*]$. Outside this strip, the boundary between D_+ and D_- is either an horizontal line $(\mu_i = |U|$ if $\mu_e < -2t - |U|$, i.e. $\rho_e = 0$, and $\mu_i = -|U|$ if $\mu_e > 2t + |U|$, i.e. $\rho_e = 1)$, or consists of curves ending at $\pm\mu_e^*$. For any (μ_e, μ_i) on these curves, the ground state is a mixture of two "pure states":

$$(\rho_i = 1, \rho_e = \rho_e^+(\mu_e)) \text{ and } (\rho_i = 0, \rho_e = 0) \text{ if } \mu_e < -\mu_e^*,$$

$$(\rho_i = 1, \rho_e = 1) \; (\rho_i = 0, \rho_e = \rho_e^-(\mu_e)) \text{ if } \mu_e < -\mu_e^*.$$

Thus the ground state is the segregated configuration (sect. 3.1) with

$$\rho_e = \alpha\rho_i < b(|U|)\rho_i \qquad \text{any} \qquad \rho_i \in [0,1] \qquad \text{if} \qquad \mu_e < -\mu_e^* \qquad (3.7)$$

and

$$\rho_e = 1 - \alpha \rho_i > 1 - b(|U|)\rho_i \qquad \text{any} \qquad \rho_i \in [0,1] \qquad \text{if} \qquad \mu_e > -\mu_e^* \qquad (3.8)$$

where α increases from 0 (for $\mu_e = -2t - |U|$) to a maximum value $b(|U|) < 1$ (for $\mu_e = \mu_e^*$) and similarly for $\mu_e > 0$. This is precisely the second conjecture discussed in section 3.1, which thus seems to be correct for all U. A formula for $\mu_e^*(U)$ and thus $b(|U|)$ was derived in [42]; it relies on a reasonable argument, but it is not a proof (see also [49] for upper and lower bounds).

Inside the strip $[-\mu_e^*, \mu_e^*]$ the domain D separates D_+ from D_-. Again all electron densities appear in D, and the ion density satisfies

$$b(|U|)\rho_i < \rho_e < 1 - b(U)\rho_i \qquad (3.9)$$

If $|U| > 2t$, then for any (μ_e, μ_i) inside D the ground state is neutral ($\rho_e = \rho_i$) and consists of neutral atoms homogeneously distributed. In this case $\rho_e = \rho_i = cte$ along the lines $\mu_e + \mu_i = cte$ in D (fig. 2b). The linear boundary between D_- and D (for $\mu_e \in [\mu_e^*, -2t + |U|]$) describes the limiting case of neutral systems with $\rho_e = \rho_i = 0$. On the other hand the curved boundary of D_- and D describes mixtures of the empty configuration ($\rho_i = 0, \rho_e \in [0, 1 - b(U)]$ with some periodic neutral configuration given by (3.1).

For $|U| < 2t$, the domain D presents a very rich and interesting structure (fig. 1b). One observes a partition of D into domains D_{ρ_e} in which the electron density has a definite rational value $\rho_e = p/q$. These domains form curved stripes going across D from the boundary with D_- to the boundary with D_+. Each domain D_{ρ_e} is further partitioned by horizontal lines into subdomains $D_{(\rho_e, \rho_i)}$, with $\rho_i = p_i/q$, $p_i \in \{p', p' + 1, ..., p''\}$, in which the ground state is given by (3.1). The horizontal boundary between p_i/q and p_{i+1}/q describes mixtures of these two periodic configurations and similarly for the boundary between D_- and $D_{(p/q, p'/q)}$ and that between $D_{(p/q, p''/q)}$ and D_+. This is the property established in the limit $U \to 0$ (sect. 3.1). Restricting the rest of the discussion to $\mu_e \leq 0$ i.e. $\rho_e \leq 1/2$ (since the case $\mu_e > 0$ is obtained by a particle-hole transformation), one also observes that D contains large connected domains D_n, $n = 1, ..., n_{max(U)}$ corresponding

to the most homogeneous configuration of $n - molecules$ consisting of n consecutive sites occupied by an ion with one electron per $n - molecule$ ($\rho_i = n\rho_e$). In particular because of (3.9) $n_{max}(U) < 1/b(U)$. In each domain D_n the electron density varies continuously between $\rho_n^{min}(U)$ and $\rho_n^{max}(U)$. The atomic domain D_1 ($\rho_e = \rho_i$) always contains the symmetry point $(0,0)$ and, as we have seen, $\rho_1^{min}(U) > 0$ for $U < t/\sqrt{3}$. On the other hand $\rho_n^{max}(U) < 1$ for $n \geq 2$. Finally it was checked that for any μ inside a domain $D_{(\rho_e, \rho_i)}$, the Fermi level μ_e lies in a gap of the corresponding spectrum and the system is an insulator. Very recent computations [] confirm these results except for the fact that for some values of $|U|$, new structures might appear between D_+ and D, as well as between D_- and D. Further computations are however necessary to draw new conclusions.

To conclude this section let us mention two types of analytical results (also valid in higher dimensions) which have been obtained in the grand canonical ensemble:

1) For any U, using Tchebycheff-Markov inequalities [12,35], it is possible to find domains $D'_+ \subset D_+$, $D'_- \subset D_-$, $D'_{cb} \subset D$ (D_{cb} contains the origin) where one can rigorously prove that the ground states are respectively the full, empty, and chessboard configurations [37,38].

2) For very large $|U|$ and μ_e in the gap $[2t - |U|, -2t + |U|]$, so that $\rho_e = \rho_i = \rho$, using the perturbation expansion (2.18) it is possible to find domains where one can prove that the ground states are the most homogeneous configurations with densities 0, 1/5, 1/4, 1/3, 2/5, 1/2, 3/5, 2/3, 3/4, 4/5, 1. This leads to the conjecture that the phase diagram (fig. 2b) has a devil staircase structure as first pointed out in [44]. Such a structure has been found in the classical Frenkel-Kontorova model [82] and the Ising model with long range interaction [83].

4. HIGHER DIMENSIONS

In two or three dimensions much less is known about the phase diagrams. Very recently the FK model on the square lattice, with nearest neighbour hopping $t_{<xy>} = t$ and no magnetic field, was investigated in the grand canonical formalism, by numerical diagonalisation of the hamiltonian [54]. Although the phase diagrams are more complex, they

present surprising similarities with the one dimensional case: general structure, segregation for $\rho_e \neq \rho_i$, only neutral homogeneous configurations for large $|U|$, molecule formation for small U, ground state configuration of ions similar to (3.1), devil staircase structure, Farey's sequence. A new feature which appears in two dimensions is the fact that for some densities $\rho = \rho_e = \rho_i$ the configuration of ions in the ground state changes as U is varied. A similar property will be discussed below where we shall see that for some densities $\rho = \rho_e = \rho_i$ the configuration of ions changes with the magnetic field (at fixed U).

The ground states are rigorously known in two dimensions for a few simple rational values of the density and in all dimensions only for the ionic densities ρ_i equal to 0, 1/2, 1. For finite temperatures one can prove the occurence of long range order of chessboard type in a neighborhood of the symmetry point. Long range order corresponding to other periodicities probably exists but has not yet been established rigorously.

4.1. Ground States : Canonical Ensemble

The problem is to find the minima of $E_N(\mathbf{s})$ given by (2.8), for the FK model.

The half filled band and neutral case for density $\rho_e = \rho_i = 1/2$

The following theorem, due to Kennedy and Lieb [14], is the first rigorous result on the subject and holds on any bipartite lattice in any dimension and any fixed flux. (In fact one can view the lattice as an abstract graph, for that theorem.) We give a generalisation to interacting spin one-half electrons and hard-core bosons in section 5 for special values of the flux using a different proof.

Theorem 4.1.

For any finite bipartite lattice $\Lambda = A \cup B$:

(i) Let $U > 0$. Under the condition $N + N_i \geq |\Lambda|$, the minimum of $E_N(\mathbf{s})$ over N and $\mathbf{s}$ is attained either for $N = |A|$, $N_i = |B|$, $s_x = -1$, $x \in A$, $s_x = +1$, $x \in B$, and for $N = |B|$, $N_i = |A|$, $s_x = +1$, $x \in A$, $s_x = -1$, $x \in B$. So we have at least two degenerate minima.

(ii) Let $U < 0$. Under the condition $N + N_i \leq 2|A|$ (resp $N + N_i \leq 2|B|$) the minimum is attained at $N = N_i = |A|$, $s_x = +1$, $x \in A$, $s_x = -1$, $x \in B$ (resp $N = N_i = |B|$, $s_x = +1$, $x \in B$, $s_x = -1$, $x \in A$). If $|A| = |B|$ we have at least two degenerate minima.

(iii) In each of the above cases these are the only minima (here it is important that Λ is connected as we assumed in the introduction).

In particular for $\Lambda \subset \mathbf{Z}^d$ the minimizing configuration is a chessboard. If the lattice satisfies $|A| = |B|$, this theorem settles the minimization over $\mathbf{s}$ under the constraint $N = |A| = |B|$, which corresponds to an electron and ion density equal to one-half.

Theorem 4.2 establishes the existence of a charge gap, under the additional condition that Λ is fully connected [14]. This means that for every $x,y \in \Lambda$ there exist a path connecting x and y such that on all bonds (a,b) of the path, $|t_{ab}| > \delta > 0$ for some fixed number δ.

Theorem 4.2.

Assume Λ bipartite and fully connected. There exist $\epsilon > 0$ depending only on $U, \delta, max|t_{xy}|$ and not on $|\Lambda|$ such that

(i) $U > 0$. There is a charge gap for $N = |A|$, $N_i = |B|$ and vice versa, i.e. $G_{N,N_i} > \epsilon > 0$.

(ii) $U < 0$. There is a charge gap for $N = N_i = |A|$ and $N = N_i = |B|$, i.e. $G_{N,N_i} > \epsilon > 0$.

One can also solve the question of the minimization with respect to the flux in certain cases. The theorem 4.3 has been proven recently in a more general context, namely that of the Hubbard model (1.1) [69] (see also [70]).

Theorem 4.3.

Take a lattice $\Lambda \subset \mathbf{Z}^d$ with periodic boundary conditions in one coordinate direction, say the horizontal one. Assume that $|t_{xy}^{(\sigma)}|$, $\sigma = \uparrow, \downarrow$, is invariant under reflections across all planes that are perpendicular to the horizontal direction cutting the cylinder in two equal halves. Then the minimum of the ground state energy over $N_\uparrow$, $N_\downarrow$ and the flux is attained for $N_\uparrow = N_\downarrow = \frac{|\Lambda|}{2}$ and $\Phi = \pi$ through all square two dimensional faces.

For the Falicov-Kimball model one applies the theorem with $t_{xy}^{(\uparrow)} = 0$. One can generalise to other lattices by letting $|t_{xy}| \to 0$, on some of the bonds, in a way which respects the assumption. Then the optimal flux is 0 through each face with $4k + 2$ sites and π for

each face with $4k$ sites. For example for an hexagonal lattice in two dimensions $\Phi = 0$ on each hexagon, for an octagonal one $\Phi = \pi$. For a one dimensional ring $\Phi = \frac{\pi}{2}(|\Lambda| - 2)$, mod 2π. Also on a cubic three dimensional lattice $\Phi = \pi$ on all square two dimensional faces.

The significance of these results is that fermions and bosons behave very differently when they are subjected to a magnetic field. For Bose systems there is a general result, the diamagnetic inequality, which states that a magnetic field always raises the ground state energy (see for example [71]). For fermions there is not such a general principle and in fact the Falicov-Kimball and Hubbard models on a cubic lattice are examples where the contrary happens, i.e. maximal flux $\Phi = \pi$ is optimal at half filling. A continuous analog of this phenomenon is not known.

Densities $\rho_i = 1/5$, $1/4$, $1/3$ (and $4/5$, $3/4$. $2/3$) in two dimensions

In the rest of this section we consider a square two dimensional lattice with all $t_{<xy>} = t$ real, and the constraint

$$N_i = N \qquad \text{if} \qquad U < 0, \tag{4.1}$$

and

$$N_i = |\Lambda| - N \qquad \text{if} \qquad U > 0, \tag{4.2}$$

i.e. we are in a neutral situation in the electron/ion point of view, and in the half filled band from the purely electronic point of view. The problem is to minimize $E_N(\mathbf{s})$ under the constraint (4.1) or (4.2). The following is due to Kennedy [56]

Theorem 4.4

For $t_{<xy>} = t$ real, $|U|$ sufficiently large, and $\rho_i = 1/5, 1/4, 1/3$ (and $4/5, 3/4, 2/3$) the minimum of $E_N(\mathbf{s})$ under the constraint (4.1)-(4.2) is attained for the three periodic configurations $\mathcal{S}_1$, $\mathcal{S}_2$, $\mathcal{S}_3$ of figure 3.

In the paragraph 4.2 we indicate how this theorem can be partly extended to non zero flux (i.e. t_{xy} complex).

For $\rho_e = \rho_i = 1/2$, we know that the chessboard configuration occurs for all U. So a natural question is whether or not the configurations of figure 3 are ground states for all

U. The numerical results obtained in one and two dimensions [42,54] point to a negative answer for small (or large) densities.

$$\mathcal{S}_1, \rho = \tfrac{1}{5} \qquad \mathcal{S}_2, \rho = \tfrac{1}{4} \qquad \mathcal{S}_3, \rho = \tfrac{1}{3}$$
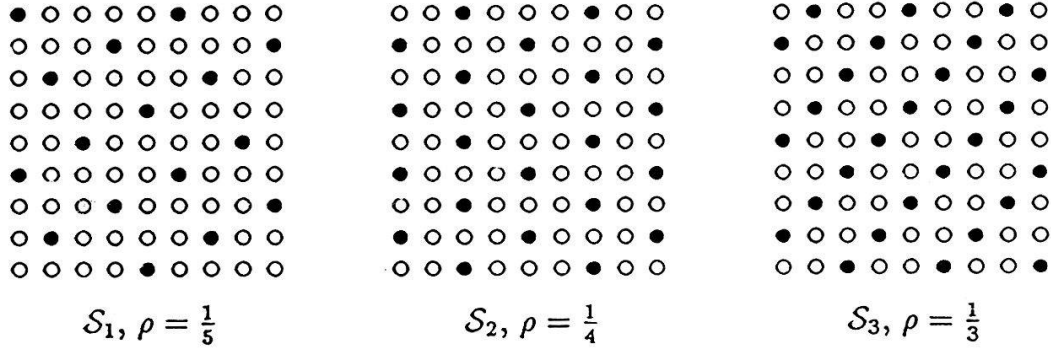
Figure 3: Ground state configurations on the *square* lattice, for $\rho_i = 1/5, 1/4, 1/3$. Ions are represented by black dots. For the complementary densities $4/5, 3/4, 2/3$ one exchanges black and white dots.

For other rational values of the density Kennedy [56] obtained the following. Let ρ_i be some rational density and suppose there exists $U_0(\rho_i)$ and a configuration $s(\rho_i)$ such that $s(\rho_i)$ is a ground state for all $|U| \geq U_0(\rho_i)$. Under some additional mild assumption on $s(\rho_i)$ when $\rho_i \in [1/3, 1/2]$ the ground states $s(\rho_i)$ consist of parallel line with slope 1 such that s_x is constant along those lines moreover on every horizontal line each pair of consecutive nuclei is separated by one or two empty sites; when $\rho_i \in [1/4, 1/3]$ then the ground state $s(\rho_i)$ consist of parallel lines with slope 2, such that s_x is constant along those lines. The numerical results of [54] indicate that this pattern is obeyed in the range $\rho_i \in [1/5, 4/5]$, but is no longer true outside this interval.

The starting point to prove the above results is the $1/U$ expansion (see sect. 1). For the hamiltonian $H_{trunc}(s)$ obtained by truncating the expansion at order U^{-3} one can find the ground states of figure 3. To this end one rewrites $H_{trunc}(s)$ as a sum over blocks B (e.g. : three by three blocks) $H_{trunc}(s) = \sum_B H_B(s)$. Suppose that we find s

which minimizes $H_B(\mathbf{s})$ for all blocks simultaneously. Then obviously this $\mathbf{s}$ is a ground state of $H_{trunc}(\mathbf{s})$. Usually it is not possible to find such an $\mathbf{s}$. In this case one tries to find another decomposition of $H_{trunc}(\mathbf{s})$. This can be done by replacing $H_B(\mathbf{s})$ by $H_B(\mathbf{s}) + K_B(\mathbf{s})$ with $\sum_B K_B(\mathbf{s}) = 0$. It is even enough to require $\sum_B K_B(\mathbf{s})$ proportional to $\sum_x s_x$ since we work at fixed ion number. This kind of idea was first used in [37] and we encounter it again in paragraph 4.2. Once the ground states of the truncated hamiltonian are known one has to show that the higher order terms do not destroy them. This necessitates the control of their magnitude and their range.

4.2. Ground States : Grand Canonical Ensemble

In this paragraph we consider the general problem of minimizing (2.22) for each (μ_e, μ_i). At the symmetry point $(\mu_e, \mu_i) = (0,0)$ the minimization is achieved by theorem 4.5 (analogous to 4.1) and yields the chessboard configurations. In fact it is also valid for the effective interaction $F_\Lambda(\mathbf{s}, \beta, 0, 0)$. In section 5 we generalise this theorem to some interacting systems for special values of the flux.

Theorem 4.5

Let $\Lambda = A \cup B$ be a bipartite lattice. Then for any given flux, the minimum of $E_\Lambda(\mathbf{s}, 0, 0)$ and $F_\Lambda(\mathbf{s}, \beta, 0, 0)$, is attained at the two configurations $s_x = \pm\epsilon_x$, $\epsilon_x = +1$, $x \in A$, $\epsilon_x = -1$, $x \in B$.

We give the argument because of its generality and simplicity. Using the unitary $\epsilon_x \delta_{xy}$ and the concavity of $tr\sqrt{X}$, for X any $|\Lambda| \times |\Lambda|$ matrix we have

$$
\begin{aligned}
tr|h_\Lambda(\mathbf{s})| &= \frac{1}{2}tr\sqrt{(T+US)^2} + \frac{1}{2}tr\sqrt{(T-US)^2} \\
&\leq tr\sqrt{T^2 + U^2}
\end{aligned} \tag{4.3}
$$

Then by (2.23)

$$
E_\Lambda(\mathbf{s}, 0, 0) \geq -\frac{1}{2}tr\sqrt{T^2 + U^2} \tag{4.4}
$$

The special configurations of theorem 4.5 always satisfy $TS + ST = 0$, and thus their energy is precisely $-\frac{1}{2}tr\sqrt{T^2 + U^2}$. So the equality is achieved in (4.4) for these configurations.

In [37,38] it was shown that the chessboard persists in a neighborhood of the symmetry point (for any dimension).

For $|U|$ large enough ($|U| >> zmax|t_{xy}|$) one can predict a more complete phase diagram by perturbative methods. In the rest of this paragraph we adress this problem for two dimensions, on a square lattice with $|t_{<xy>}| = t$ and constant magnetic flux Φ through each 2×2 plaquette.

To this end one uses the U^{-1} expansion ($U > 0$) for μ_e in the gap [55]

$$
\begin{aligned}
E(\mathbf{s}, \mu_e, \mu_i) = &\frac{1}{2}(\mu_e - \mu_i) \sum_x s_x + (\frac{t^2}{4U} - \frac{t^4}{16U^3}(7 + 2\cos\Phi)) \sum_{|x-y|=1} s_x s_y \\
&+ \frac{t^4}{16U^3}(4 - \cos\Phi) \sum_{|x-y|=\sqrt{2}} s_x s_y + \frac{t^4}{8U^3} \sum_{|x-y|=2} s_x s_y \\
&+ \frac{5t^4}{16U^3} \cos\Phi \sum_P \prod_{x \in P} s_x + \frac{t^4}{16U^3} \cos\Phi \sum_P 1 + O(U^{-5})
\end{aligned}
\tag{4.5}
$$

where the double sums are on pairs $\{x, y\} \subset \Lambda$ and the last sum is over the 2×2 plaquettes in Λ. Using the method explained in sect. 4.1, the phase diagram of figure 4 was obtained [55] for the truncated hamiltonian where the terms of order U^{-5} in (4.5) are neglected.

The phase diagram is symmetric with respect to $\mu \to -\mu$ (here $\mu = \mu_e - \mu_i$) as can be seen from (4.5). Here $\mathcal{S}_1, \mathcal{S}_2, \mathcal{S}_3$ correspond to the configurations of figure 3, $\overline{\mathcal{S}}_1, \overline{\mathcal{S}}_2, \overline{\mathcal{S}}_3$ are the complementary ones, $\mathcal{S}_{cb}$ is the chessboard, $\mathcal{S}_-, \mathcal{S}_+$ the empty and full configurations. The three lines separating phases 1/5, 1/4, 1/3 are infinitely degenerate and are given by equating the corresponding energies. If one would neglect the terms of order U^{-3} in (4.5) the phase diagram is that of the antiferromagnetic Ising model: the two vertical dotted lines correspond to a family of infinitely degenerate ground states. When the terms of order U^{-3} are included this degeneracy is lifted leading to new regions of smaller width in figure 4. We expect that the degenerate lines open up again when higher order terms are taken into account. Probably a devil staircase structure appears in the limit of an infinite number of terms. Having obtained the ground states of the hamiltonian truncated at order U^{-5}, one can show that the rest of the expansion does not modify this phase diagram except around the boundaries (where the devil staircase will take place).
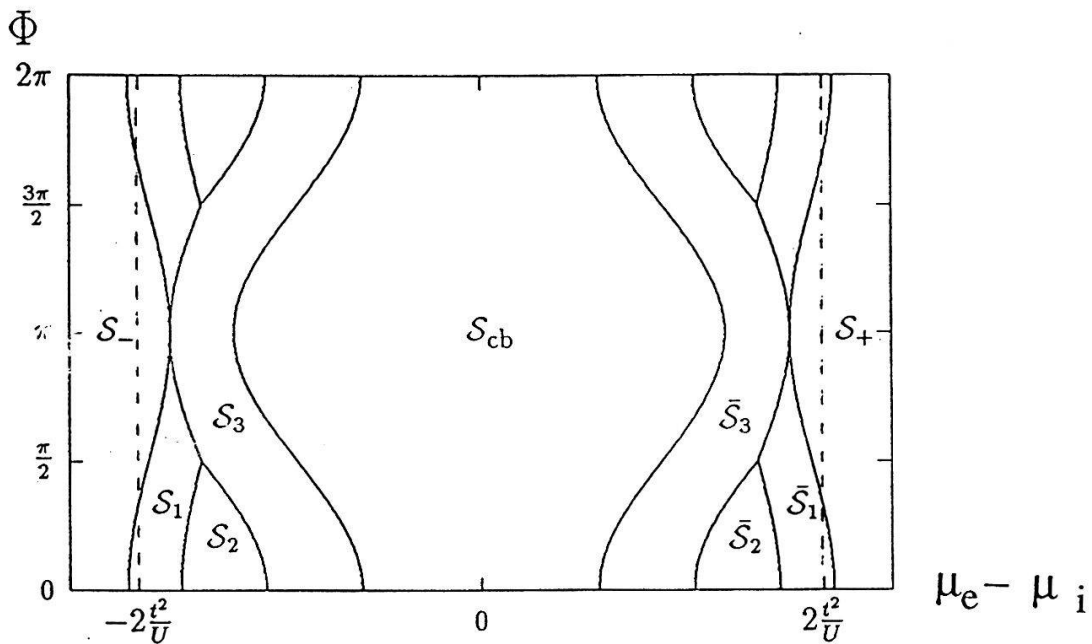
Figure 4: Phase diagram to order U^{-3} in the $(\mu_e - \mu_i, \Phi)$ plane, for a *square* lattice, and with *Fermi* statistics. The dotted lines correspond to the phase diagram of the Ising model obtained to order U^{-1}.

These results provide an extension of theorem 4.4 to the case of fixed non zero homogeneous flux, for $\Phi \notin [\frac{\pi}{2}, \frac{3\pi}{2}]$. For $\Phi \in [\frac{\pi}{2}, \frac{3\pi}{2}]$, and $\Phi \neq \pi$, the ground state configurations are rigorously established for densities $\rho_i = 1/5, 1/3, 1/2$. For $\Phi = \pi$ only $\rho_i = 1/3, 1/2$ are rigorously known.

For all the rigorously established configurations it appears that, given a density the configuration is unique and independent of the flux. Our guess is that this is always true on a square lattice if U is large enough. As will be seen below it is not the case on the triangular lattice.

If we plot the electron density as a function of the chemical potential for a fixed value of the flux we see plateaux in finite intervals of chemical potential. Physically this means that the system is incompressible and that the ground state energy as a function of the density has cusps at the densities $1/5, 1/4, 1/3, 1/2$ (and the complementary ones).

A similar study can be achieved also for the triangular lattice. This is not a bipartite lattice and therefore one might expect that qualitatively different features appear.

For example the particle-hole symmetry is lost and this is clearly reflected in the phase diagram. Here we summarise the results in order to show what are the qualitative differences with the square lattice.

In [55] a U^{-1} expansion is derived up to order U^{-3}. To order U^{-1} we get the Ising hamiltonian, and there are terms of order U^{-2}, in contrast to (4.5), which break the spin flip symmetry. To this order the phase diagram can be analysed exactly, and is plotted on figure 5. The configurations $\mathcal{T}_-$, $\mathcal{T}_+$ correspond to the empty and full lattice, while $\mathcal{T}_5$, $\overline{\mathcal{T}}_5$ have density 1/3, 2/3 (see fig. 6) and correspond to those of the Ising model with a small magnetic field.
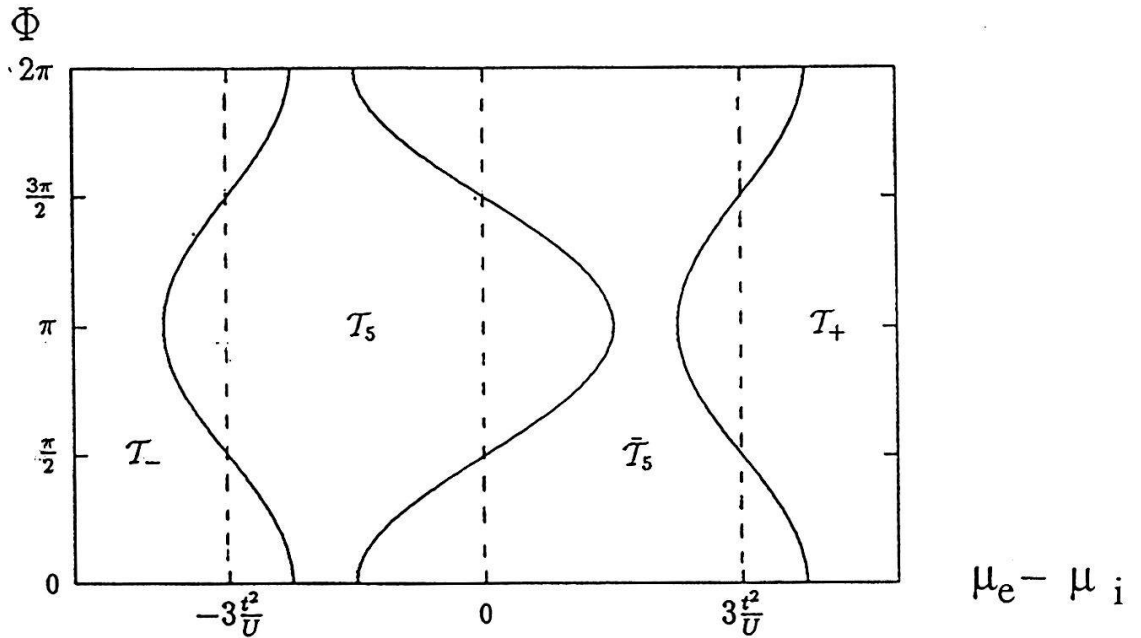

Figure 5: Phase diagram to order U^{-2} in the $(\mu_e - \mu_i, \Phi)$ plane, for a *triangular* lattice, and with *Fermi* statistics. The dotted lines correspond to the phase diagram of the Ising model obtained to order U^{-1}.

To order U^{-3} the lines separating the different phases open up and a variety of new configurations appear. The phase diagram becomes complicated and we refer to [55] for the details. Here we just mention one interesting feature. There exist regions in the $(\mu_e - \mu_i, \Phi)$ plane corresponding to densities 1/4 and 1/2 where the ground states are those of figure

6, and it appears that given a density (1/4 or 1/2) the configuration changes (from $\mathcal{T}_3$ to $\mathcal{T}_4$ or from $\mathcal{T}_8$ to $\mathcal{T}_9$ as the flux is varied. As said before, on the square lattice this does not seem to occur, and therefore the effect might be related to the fact that the triangular lattice is not bipartite.

Finaly we note that for a flux $\Phi = \pi/2$ or $3\pi/2$ per triangle the particle-hole symmetry is recovered and therefore for these fluxes the phase diagram is symmetric around $\mu_e - \mu_i = 0$, to all order of perturbation theory.
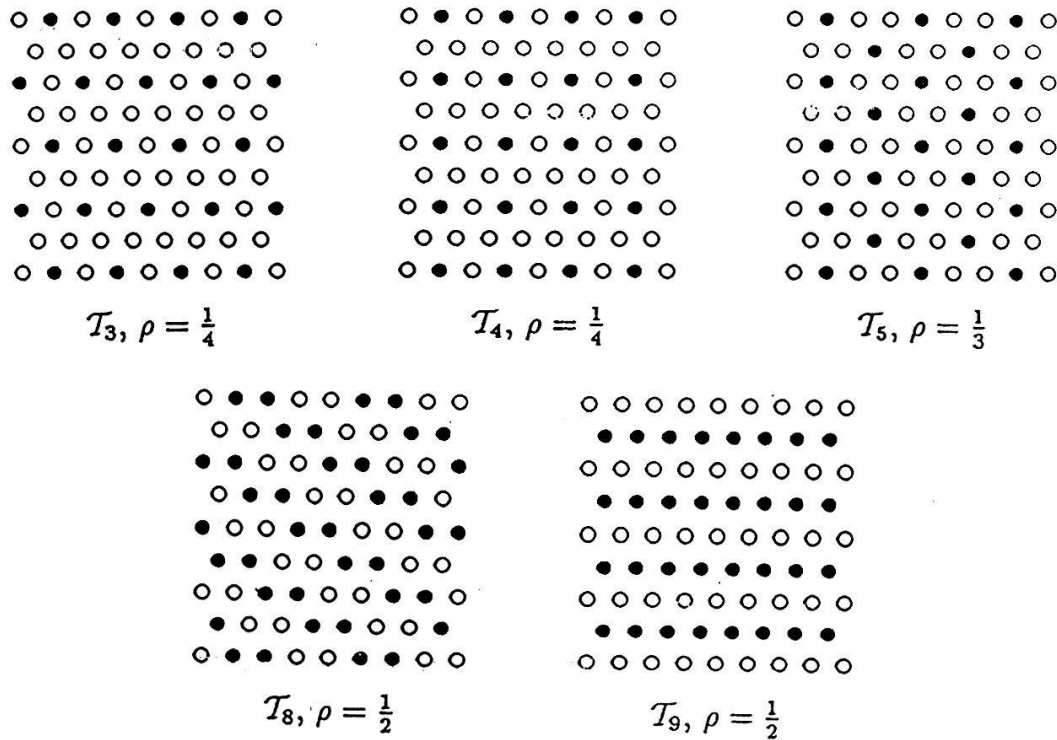

Figure 6: Ground state configurations on the *triangular* lattice, for $\rho_i = 1/4, 1/3, 1/2$. Ions are represented by black dots.
For the complementary densities $3/4, 2/3, 1/2$ one exchanges black and white dots.

4.3. Low Temperature Phase Diagram

For finite temperatures the stability of the chessboard phase at low temperature has been studied on $\mathbf{Z}^d$, $d \geq 2$, for $t_{xy} = t$ real (i.e. zero flux). These results which we describe below can be extended straightforwardly to non zero flux.

At the symmetry point, Kennedy and Lieb succeeded to analyse the phases of the model for all values of U [14].

In this situation the density of electrons and nuclei are both equal to 1/2 at all temperatures.

There exist $\beta_l(U)$ with $\beta_l(U) \simeq |U|^{-2}|\ln U|$ for $U \to 0$ and $\beta_l(U) \simeq c_2|U|$ for $U \to \infty$, such that for $\beta > \beta_l(U)$ the low temperature phase is characterised by

$$(-1)^{|x|+|y|} < s_x s_y >_\Lambda \geq c > 0 \tag{4.6}$$

for some constant c, independent of x and y and Λ. In (4.6) periodic or free boundary conditions are used to define $< - >_\Lambda$. Choosing appropriate boundary conditions we can select the two pure phases corresponding to the two chessboard ground states.

Moreover there exist $\beta_h(U)$ with $\beta_h(U) \simeq |U|^{-1/(d+2)}$ for $U \to 0$ and $\beta_h(U) \simeq c_1|U|$, for $U \to \infty$, such that for $\beta < \beta_h(U)$ the high temperature phase is characterised by the exponential decay of correlations

$$| < s_x s_y >_\Lambda | \leq C \exp(-m|x - y|) \tag{4.7}$$

with C and m positive, independent of x, y and $|\Lambda|$.

We do not expect that other phases separate the high and low temperature behaviour. This picture is confirmed by the exact solution of the Falicov-Kimball model at half filling in the limit of infinite dimension, where a single line $\beta_c(U)$ separates the high and low temperature phases [23]. It is found that $\beta_c(U) \simeq U^{-2}|lnU|^{-1}$ for $U \to 0$ and $\beta_c(U) \simeq cU$ for $U \to \infty$. This behavior for $U \to \infty$ holds in fact in all dimensions since $\beta_l(U)$ and $\beta_h(U)$ are asymptotically linear for large U.

From the U^{-1} expansion it is expected that the model behaves as an Ising antiferromagnet for large U. The proof given in [14] involves a non trivial adaptation of the Peierls argument. Here unlike in the Ising hamiltonian the energy of a spin configuration is not given explicitly so that the hard part consists in proving that one gains a positive energy by removing a Peierls contour. More precisely if $\mathbf{s}$ contains a Peierls contour γ, and $\mathbf{s}^*$ is obtained by a spin flip transformation inside γ, one proves that

$$F_\Lambda(\mathbf{s}, \beta, 0, 0) - F_\Lambda(\mathbf{s}^*, \beta, 0, 0) \geq C(\beta, U)|\gamma| \tag{4.8}$$

where $|\gamma|$ is the lenght of the contour and the positive constant is independent of $|\Lambda|$, $\mathbf{s}$, $\mathbf{s}^*$, and $\beta C(\beta, U) >> 1$ for large β. To obtain (4.8) one has to decouple the interior (int) and

exterior (ext) of γ. Formally $F_\Lambda(\mathbf{s}, \beta, 0, 0)$ is represented as a sum of three corresponding terms $F_\Lambda^{ext}(\mathbf{s}) + F_\Lambda^{int}(\mathbf{s}) + F_\Lambda^\gamma(\mathbf{s})$, the last one representing the energy cost of the boundary of γ. The unitary $\epsilon\delta_{xy}$, which leads to the invariance of $F_\Lambda(\mathbf{s}, \beta, 0, 0)$ under $\mathbf{s} \to -\mathbf{s}$, then implies $F_\Lambda^{ext,int}(\mathbf{s}) = F_\Lambda^{ext,int}(\mathbf{s}^*)$ and thus the difference in the left hand side of (4.8) is $F_\Lambda^\gamma(\mathbf{s}) - F_\Lambda^\gamma(\mathbf{s}^*) = O(|\gamma|)$.

Around the symmetry point, keeping only the leading orders in (4.5), the hamiltonian for large U is that of the Ising antiferromagnet with nearest neighbour coupling constant $t^2/4U$ and a magnetic field $\frac{1}{2}(\mu_e - \mu_i)$. Thus one expects that the antiferromagnetic long range order is preserved for $|\mu_e - \mu_i| = O(U^{-1})$ with $|\mu_e| < U - 4t$, since the U^{-1} expansion is valid for μ_e in the gap. We note that for finite temperatures the density is no longer fixed to 1/2 for finite temperatures. Also the effective potential is not invariant under a global spin flip. It turns out that the special transformation $\mathbf{s} \to \mathbf{s}^*$ found by Dobrushin [72,73] for the Ising antiferromagnet with a magnetic field is well adapted to the present situation. The procedure is to erase the upper interior line of spins along the upper boundary of γ, to translate the configuration inside γ by one lattice site in the upper direction, and to flip the last line of spins along the lower interior boundary of γ. Then (4.8) was proved in [34] for (μ_e, μ_i) in a strip

$$\Sigma = \{(\mu_e, \mu_i) \mid |\mu_e + \mu_i| = o(U), |\mu_e - \mu_i| = O(U^{-1})\} \tag{4.9}$$

U large and $C(\beta, U) = U^{-1}$. Using this result it is straightforward to generalise (4.6) to $(\mu_e, \mu_i) \in \Sigma$, β/U and U large. The reason that Dobrushin's transformation can be used successfully is that it can be represented in the Hilbert space of wave functions by an approximately unitary transformation. This is clear if one thinks of large contours where $\mathbf{s} \to \mathbf{s}^*$ is a "translation up to boundary terms". We have in this case $F_\Lambda^{ext}(\mathbf{s}) = F_\Lambda^{ext}(\mathbf{s}^*)$, $F_\Lambda^{int}(\mathbf{s}) = F_\Lambda^{int}(\mathbf{s}^*) + O(|\gamma|)$.

It is expected that the other ground states found in fig. 3 correspond also to stable low temperature states. However the Peierls-Dobrushin argument used at, or near, the symmetry point breaks down for obvious geometrical reasons (see fig. 3) and thus Pirogov-Sinai theory should be applied. However a good control of the potentials $J_X(\beta, \mu_e, \mu_i)$ appearing in (2.29) is needed. An interesting method to obtain results in this direction

has been devised by A. Messager and S. Miracle-Sole [57]. The classical weight of the $d-$ dimensional model $\exp(-\beta F_\Lambda)$ is represented, via a functional integral formulation, as the partition function of a polymer system in $d+1$ dimensions. At low temperatures and large U the polymer system is dilute and standard cluster expansion techniques of classical statistical mechanics can be applied. One can then get some information on the structure of (2.29). In [57] the authors recover the results on the stability of the chessboard phase near the symmetry point. This technique is also very useful to treat the case of hard-core bosonic systems (sect. 5).

5. INTERACTING SYSTEMS

In this section we consider two types of interacting systems. The first one is a bosonic model with hamiltonian (2.5) where $a_x^\dagger$, a_y are replaced by hard-core Bose operators $b_x^\dagger$, b_y satisfying

$$b_x^\dagger b_x + b_x b_x^\dagger = 1, \qquad (b_x^\dagger)^2 = (b_x)^2 = 0 \tag{5.1}$$

and

$$b_x^\dagger b_y - b_y b_x^\dagger = b_x b_y - b_y b_x = 0, \qquad x \neq y \tag{5.2}$$

Since two bosons cannot occupy the same lattice site, we can imagine that they interact by a repulsive two body on-site potential $\lambda b_x^\dagger b_x (b_x^\dagger b_x - 1)$ with $\lambda \to \infty$. The algebra (5.1), (5.2) can be represented explicitly by the Pauli matrices

$$\tau^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \tau^2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \qquad \tau^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{5.3}$$

thanks to the identification $b_x^\dagger = \frac{1}{2}(\tau^1 - i\tau^2)$, $b_x = \frac{1}{2}(\tau^1 + i\tau^2)$, and $b_x^\dagger b_x = \frac{1}{2}(\tau^3 + 1)$.

The second type of model is given by the hamiltonian (2.7) for fermions with spin one-half, or for hard-core bosons with "spin one-half" (i.e. two kinds of hard-core Bose particles).

5.1. Reflection Positivity

We briefly state a basic inequality needed later. Let $\mathcal{H}$ be a d dimensional Hilbert space and A, B, C_i, $i = 1, ..., n$, $d \times d$ matrices with A, B hermitian and C_i real. Let $\mathcal{H} \otimes \mathcal{H}$

be the usual tensor product and set for any $d \times d$ matrix D, $D = D \otimes \mathbf{1}$, $\tilde{D} = \mathbf{1} \otimes D$, and $D^* = D^* \otimes \mathbf{1}$, $\tilde{D}^* = \mathbf{1} \otimes D^*$, where $*$ is the ordinary complex conjugation (not hermitian conjugation). Suppose also that $\sum_i \gamma_i (C_i - \tilde{C}_i)^2$ is symmetric, where γ_i are real numbers. If $\gamma_i \geq 0$ for all i, then for any real h_i the Cauchy-Schwartz inequality implies [74]

$$Tr \exp[A + \tilde{B}^* - \sum_{i=1}^n \gamma_i (C_i - \tilde{C}_i - h_i)^2] \leq \left(Tr \exp[A + \tilde{A}^* - \sum_{i=1}^n \gamma_i (C_i - \tilde{C}_i)^2] \right)^{1/2}$$
$$\times \left(Tr \exp[B + \tilde{B}^* - \sum_{i=1}^n \gamma_i (C_i - \tilde{C}_i)^2] \right)^{1/2}$$
(5.4)

In the applications of (5.4), it is important to realize that the matrices D and $\tilde{D}$ commute. The idea will be to write the hamiltonian in the form

$$-A - \tilde{B}^* + \sum_{i=1}^n \gamma_i (C_i - \tilde{C}_i - h_i)^2, \qquad \gamma_i \geq 0$$
(5.5)

and to apply the inequality (5.4). Note that the plus sign in front of the sum of squares in (5.5) is crucial. If the hamiltonian can be written in the form (5.5), (possibly after some transformations leaving $Tr \exp(-\beta H_\Lambda)$ invariant) we say that it has the reflection positivity property (RP). However this property refers to a particular tensor product decomposition of the Hilbert space, so that (5.5) may not be unique. We give two examples below: reflection positivity in *spin space* and in *position space*.

Reflection positivity in spin space

Suppose that we have spin one-half fermions or spin one-half hard-core bosons such that the number of spin down and spin up particles is the same. Then one can view the Hilbert space as $\mathcal{H}_\uparrow \otimes \mathcal{H}_\downarrow$, with $\mathcal{H}_\uparrow$, $\mathcal{H}_\downarrow$ two identical copies of the same $\mathcal{H}$. If we denote by $a^\dagger$, a, (or $b^\dagger$, b) the creation and annihilation operators in $\mathcal{H}$ we can rewrite (2.7) as

$$H_\Lambda(\mathbf{s}) = - \sum_{x,y \in \Lambda} t_{xy} (a_x^\dagger a_y \otimes \mathbf{1} + \mathbf{1} \otimes a_x^\dagger a_y) + U \sum_{x \in \Lambda} s_x [(a_x^\dagger a_x - \frac{1}{2}) \otimes \mathbf{1} + \mathbf{1} \otimes (a_x^\dagger a_x - \frac{1}{2})]$$
$$+ U' \sum_{x \in \Lambda} (a_x^\dagger a_x - \frac{1}{2}) \otimes (a_x^\dagger a_x - \frac{1}{2})$$
(5.6)

Since

$$(a_x^\dagger a_x - \frac{1}{2}) \otimes (a_x^\dagger a_x - \frac{1}{2}) =$$
$$-\frac{1}{2}\left[(a_x^\dagger a_x - \frac{1}{2}) \otimes \mathbf{1} - \mathbf{1} \otimes (a_x^\dagger a_x - \frac{1}{2})\right]^2 + \frac{1}{4}\mathbf{1} \otimes \mathbf{1} \tag{5.7}$$

we see that (5.6) is RP in spin space for any lattice and for $U' \le 0$, t_{xy} hermitian, all U, all $\mathbf{s}$. Following the methods of [75] one can then prove that the hamiltonian (2.7) for spin one-half fermions and for hard-core bosons has among its ground states at least one singlet state for any lattice provided $U' \le 0$.

Reflection positivity in position space

Let us consider a cubic d-dimensional lattice with periodic boundary conditions in a selected coordinate direction δ (so we have a cylinder). We select an hyperplane Π_δ perpendicular to the δ direction separating the cylinder into a left (L) and a right (R) part, with the same number of sites on both sides. For a bosonic system the Hilbert space can be viewed as $\mathcal{H}_L \otimes \mathcal{H}_R$, where $\mathcal{H}_{L,R}$ are the Fock spaces associated to the left and right parts of the lattice. These are two identical copies of the same space $\mathcal{H}$. Moreover this construction can be applied with respect to any hyperplane Π_δ perpendicular to the δ direction, and separating the system in two equal parts.

For fermion systems, given Π_δ we first perform the transformation*

$$\hat{a}_{x\sigma}^\dagger = e^{i\pi N_L} a_{x\sigma}^\dagger, \qquad x \in \Lambda \tag{5.8}$$

where $N_L = \sum_{x \in L} \sum_\sigma a_{x\sigma}^\dagger a_{x\sigma}$, L the left part of the lattice [70]. This transformation ressembles the one-dimensional Jordan-Wigner transformation but it is different. One can check that the algebra of operators $\hat{a}$ on the left commutes with the algebra of operators $\hat{a}$ on the right. Therefore we can represent the Hilbert space of the fermionic states as $\mathcal{H}_L \otimes \mathcal{H}_R$, where $\mathcal{H}_L$ and $\mathcal{H}_R$ are obtained by applying the $\hat{a}^\dagger$'s on the left and right vaccuum.

---

* here it is important to note that (5.8) holds for all sites of the lattice

For hard-core bosons, the hamiltonian (2.7) can be written, after a particle-hole transformation on the right $b^\dagger_{x\sigma} \to b_{x\sigma}$, $x \in R$,

$$H_\Lambda(\mathbf{s}) \to \tilde{H}_\Lambda(\mathbf{s}) = - \sum_{x,y \in L} t_{xy} b^\dagger_{x\sigma} b_{y\sigma} + U \sum_{x \in L} s_x (b^\dagger_{x\sigma} b_{x\sigma} - \frac{1}{2})$$

$$+ U' \sum_{x \in L} (b^\dagger_{x\uparrow} b_{x\uparrow} - \frac{1}{2})(b^\dagger_{x\downarrow} b_{x\downarrow} - \frac{1}{2})$$

$$- \sum_{x,y \in R} t^*_{xy} b^\dagger_{x\sigma} b_{y\sigma} + U \sum_{x \in R} (-s_x)(b^\dagger_{x\sigma} b_{x\sigma} - \frac{1}{2}) + U' \sum_{x \in R} (b^\dagger_{x\uparrow} b_{x\uparrow} - \frac{1}{2})(b^\dagger_{x\downarrow} b_{x\downarrow} - \frac{1}{2})$$

$$+ \frac{1}{2} \left[\sum_{x \in L, y \in R} t_{xy} (b^\dagger_{x\sigma} - b^\dagger_{y\sigma})^2 + \sum_{x \in R, y \in L} t_{xy} (b_{x\sigma} - b_{y\sigma})^2 \right]$$

$$(5.9)$$

Now assume $t_{xy} = t > 0$ on all bonds cutting Π_δ. Then (5.9) is of the form

$$-A - \tilde{B}^* + \sum_i \gamma_i (C_i - \tilde{C}_i)^2, \qquad \gamma_i \geq 0 \tag{5.10}$$

with A and $\tilde{B}^*$ equal to the sums on L and R respectively and $C_i = b^\dagger_{x\sigma}, b_{y\sigma}$, $\tilde{C}_i = b^\dagger_{y\sigma}, b_{x\sigma}$, $\gamma_i = t_{xy}$, i runs over the horizontal bonds cutting Π_δ. Thus we conclude that we have RP for $t_{xy} = t > 0$, $(x, y) \cap \Pi_\delta \neq \emptyset$. The same construction can be made for other bipartite lattices (for example the hexagonal planar lattice).

For fermions using (5.8) and the electron-hole transformation on the right $\hat{a}^\dagger_{x\sigma} \to \epsilon_x \hat{a}_{x\sigma}$, $x \in R$, we find

$$H_\Lambda(\mathbf{s}) \to \tilde{H}_\Lambda(\mathbf{s}) = - \sum_{x,y \in L} t_{xy} \hat{a}^\dagger_{x\sigma} \hat{a}_{y\sigma} + U \sum_{x \in L} s_x (\hat{a}^\dagger_{x\sigma} \hat{a}_{x\sigma} - \frac{1}{2})$$

$$+ U' \sum_{x \in L} (\hat{a}^\dagger_{x\uparrow} \hat{a}_{x\uparrow} - \frac{1}{2})(\hat{a}^\dagger_{x\downarrow} \hat{a}_{x\downarrow} - \frac{1}{2})$$

$$- \sum_{x,y \in R} t^*_{xy} \hat{a}^\dagger_{x\sigma} \hat{a}_{y\sigma} + U \sum_{x \in R} (-s_x)(\hat{a}^\dagger_{x\sigma} \hat{a}_{x\sigma} - \frac{1}{2}) + U' \sum_{x \in R} (\hat{a}^\dagger_{x\uparrow} \hat{a}_{x\uparrow} - \frac{1}{2})(\hat{a}^\dagger_{x\downarrow} \hat{a}_{x\downarrow} - \frac{1}{2})$$

$$+ \frac{1}{2} \left[\sum_{x \in L, y \in R} \epsilon_y t_{xy} (\hat{a}^\dagger_{x\sigma} - \hat{a}^\dagger_{y\sigma})^2 + \sum_{x \in R, y \in L} \epsilon_x t_{xy} (\hat{a}_{x\sigma} - \hat{a}_{y\sigma})^2 \right]$$

$$(5.11)$$

If $t_{xy}\epsilon_y = t > 0$ (resp. $t_{xy}\epsilon_x = t > 0$) on bonds cutting Π_δ with $x \in L$, $y \in R$ (resp. $x \in R$, $y \in L$) we see that (5.11) is of the form (5.10), and again the hamiltonian has the RP property. This construction can also be adapted to other bipartite lattices [70].

So far we have shown that the hamiltonians of interest are RP for a special choice of the hyperplane Π_δ. However, in general, applications require that this property holds for all hyperplanes separating Λ in two equal halves, and this imposes some conditions on the hopping elements t_{xy}. In the rest of this section we give two such applications.

Application to ground state configurations $\mu_e = \mu_i = 0$

We sketch the argument for fermions on $\Lambda \subset \mathbf{Z}^d$. We take periodic boundary conditions in all directions of the lattice, and fix the flux per plaquette equal to π. Moreover we fix the flux through non trivial loops around the torus equal to π (resp 0) if the length of the loop (number of sites) is $4k$ (resp $4k + 2$).

Then, given a direction δ, (say the horizontal one) we choose a gauge such that $t_{xy}\epsilon_y = t > 0$ on bonds $< xy >$ parallel to the δ direction, and $t_{xy} = t$ on all other perpendicular bonds. Given Π_δ we view the spin configuration $\mathbf{s} = \{\mathbf{s}_L, \mathbf{s}_R\}$ as having a left part $\mathbf{s}_L$ and a right part $\mathbf{s}_R$. The effective potential in (2.27), at the symmetry point (which is the same as in sect. 2), is denoted by $F_\Lambda(\mathbf{s}) = F_\Lambda(\mathbf{s}_L, \mathbf{s}_R)$. From (5.11) we have

$$
\begin{aligned}
Tr \exp(-\beta H_\Lambda(\mathbf{s})) &= \exp(-\beta F_\Lambda(\{\mathbf{s}_L, \mathbf{s}_R\})) \\
&= Tr \exp[\beta A(\mathbf{s}_L) + \beta \tilde{A}(-\mathbf{s}_R)^* - \beta \sum_i \gamma_i (C_i - \tilde{C}_i)^2]
\end{aligned} \tag{5.12}
$$

where

$$
A(\mathbf{s}_L) = - \sum_{x,y \in L} t_{xy} \hat{a}^\dagger_{x\sigma} \hat{a}_{y\sigma} + U \sum_{x \in L} s_x (\hat{a}^\dagger_{x\sigma} \hat{a}_{x\sigma} - \frac{1}{2}) + U' \sum_{x \in L} (\hat{a}^\dagger_{x\uparrow} \hat{a}_{x\uparrow} - \frac{1}{2})(\hat{a}^\dagger_{x\downarrow} \hat{a}_{x\downarrow} - \frac{1}{2}) \tag{5.13}
$$

$$
\tilde{A}(\mathbf{s}_R) = - \sum_{x,y \in R} t_{xy} \hat{a}^\dagger_{x\sigma} \hat{a}_{y\sigma} + U \sum_{x \in R} s_x (\hat{a}^\dagger_{x\sigma} \hat{a}_{x\sigma} - \frac{1}{2}) + U' \sum_{x \in R} (\hat{a}^\dagger_{x\uparrow} \hat{a}_{x\uparrow} - \frac{1}{2})(\hat{a}^\dagger_{x\downarrow} \hat{a}_{x\downarrow} - \frac{1}{2}) \tag{5.14}
$$

and $C_i = \hat{a}^\dagger_{x\sigma}$, $\hat{a}_{y\sigma}$, $\tilde{C}_i = \hat{a}^\dagger_{y\sigma}$, $\hat{a}_{x\sigma}$, $\gamma_i = t > 0$, i is the bond (x, y) intersecting Π_δ. Then the inequality (5.4) implies

$$
\begin{aligned}
F_\Lambda(\{\mathbf{s}_L, \mathbf{s}_R\}) &\geq \frac{1}{2}(F(\{\mathbf{s}_L, -\mathbf{s}_L\}) + F(\{\mathbf{s}_R, -\mathbf{s}_R\})) \\
&\geq min(F(\{\mathbf{s}_L, -\mathbf{s}_L\}), F(\{\mathbf{s}_R, -\mathbf{s}_R\}))
\end{aligned} \tag{5.15}
$$

Thus either $\{\mathbf{s}_L, -\mathbf{s}_L\}$ or $\{\mathbf{s}_R, -\mathbf{s}_R\}$ has a lower energy than $\{\mathbf{s}_L, \mathbf{s}_R\}$. By applying successively this inequality with respect to all hyperplanes Π_δ, for each direction sucessively,

we arrive at the conclusion that the chessboard configuration must minimize the effective potential at the symmetry point, for all temperatures. The same result holds for $\beta = \infty$.

For hard-core bosons the proof works for flux 0 per square since then one can choose a gauge $t_{xy} = t > 0$ on all bonds $< xy >$.

These results generalise theorem 4.1 to interacting spin one-half fermions and hard-core bosons and are formulated in the following theorem

Theorem 5.1

Consider the hamiltonians (2.5) or (2.7) with $|t_{xy}| = t$ for hard-core bosons or fermions, on a lattice $\Lambda \subset \mathbf{Z}^d$, $d \geq 1$, with periodic boundary conditions in all directions. Set $\epsilon_x = 1$ for $x \in A$ and $\epsilon_x = -1$ for $x \in B$. We suppose

(a) *Boson case*: the flux is zero through two dimensional square faces and non trivial loops.

(b) *Fermion case*: the flux is π through two dimensional square faces and loops of length $4k$ around the torus; the flux is 0 through loops of length $4k + 2$.

Then $F_\Lambda(\beta, \mathbf{s}, 0, 0)$ attains its minimum for the two configurations $\epsilon_x s_x = \pm 1$. It is also the case for the ground state energy $E_\Lambda(\mathbf{s}, 0, 0) = \lim_{\beta \to \infty} F_\Lambda(\beta, \mathbf{s}, 0, 0)$.

Remark: This theorem can be generalised in two directions. First if $\Lambda \subset \mathbf{Z}^d$ and $|t_{xy}|$ is not uniform: the theorem holds if $|t_{xy}|$ is invariant under reflections through any reflection plane Π_δ. This generalisation is related to the Peierls instability. This connexion appears in [76] for one dimensional rings, and is discussed in [77] for two dimensions. Second, if Λ is any bipartite lattice (such as hexagonal, octagonal) with the required symmetry to apply RP. The theorem holds for bosons if we assume that the flux is zero and for fermions if we assume it is 0 through elementary faces with $4k + 2$ sites and π through elementary faces with $4k$ sites.

The optimal flux

We can now apply the above ideas to find the optimal flux for the hamiltonian (2.7). The arguments sketched below also provide a proof for theorem 4.3. The point of view outlined here clarifies the proof in [69] and has been developed in detail in [70]. Let us consider a square two dimensional lattice with periodic boundary conditions in one

direction δ (say the horizontal one). We denote by $H[\{t_{xy}\}]$ the hamiltonian for a given set $\{t_{xy}\}$ of hoppings and, for a given Π_δ, $\{t_{xy}^L\}$, $\{t_{xy}^R\}$ the hopping elements on the left and on the right parts of the lattice. Starting with (5.11) we further transform $s_x \to -s_x$ for $x \in R$. We can always choose a gauge such that $t_{xy}\epsilon_y = t > 0$ on the bonds cutting Π_δ and oriented in the δ direction. Then

$$
\begin{aligned}
Z_\Lambda &= \sum_{\mathbf{s}} Tr \exp(-\beta H_\Lambda[\{t_{xy}\}]) \\
&= \sum_{\mathbf{s}} Tr \exp\Bigg[-\beta H_L[\{t_{xy}^L\}] - \beta H_R[\{t_{xy}^R\}]^* \\
&\quad + \frac{\beta}{2} \sum_{x \in L, y \in R} |t_{xy}|(\hat{a}_{x\sigma}^\dagger - \hat{a}_{y\sigma}^\dagger)^2 + \frac{\beta}{2} \sum_{x \in R, y \in L} |t_{xy}|(a_{x\sigma}^\dagger - a_{y\sigma}^\dagger)^2 \Bigg]
\end{aligned}
\tag{5.16}
$$

where H_L and H_R are the hamiltonians corresponding to the left and right sums in (5.11). From the inequality (5.4) we have $Z_\Lambda^2 \le Z_L Z_R$ where Z_L is obtained from (5.16) by replacing $\{t_{xy}^R\}$ by $\{t_{xy}^L\}$ and Z_R by replacing $\{t_{xy}^L\}$ by $\{t_{xy}^R\}$ in Z_Λ. Thus $Z_\Lambda \le max(Z_L, Z_R)$. Let P_δ denote the plaquettes intersecting Π_δ. One can then see that in Z_L and Z_R, the flux through the plaquettes P_δ is π. By iterating the procedure with Z_L or Z_R replacing Z_Λ we arrive at the result that flux π in all plaquettes maximises Z_Λ. Taking the zero temperature limit we conclude that it minimizes the ground state energy. For more details and generalisations to other lattices we refer the reader to [70].

We also remark that for hard-core bosons the same type of proof shows that the optimal flux is zero through all plaquettes, but this follows also from more general considerations.

5.2. Bosonic Falicov-Kimball Model

The previous reflection positivity technique yields results only at the symmetry point. For hard-core spinless bosons with the "interacting" hamiltonian (2.5) the expansion methods of section 2 are not valid. However using the functional representation mentionned at the end of section 4, we can obtain the U^{-1} expansion which is convergent at least for $U > Ct$ and $|\mu_e| < U - Ct$. For the two dimensional square lattice one can take $C = 16$

and we have [55],

$$
\begin{aligned}
E(\mathbf{s}, \mu_e, \mu_i) = & \frac{1}{2}(\mu_e - \mu_i) \sum_x s_x + \left(\frac{t^2}{8U} - \frac{t^4}{16U^3}(7 - 2\cos\Phi)\right) \sum_{|x-y|=1} s_x s_y \\
& + \frac{t^4}{16U^3}(4 + \cos\Phi) \sum_{|x-y|=\sqrt{2}} s_x s_y + \frac{t^4}{8U^3} \sum_{|x-y|=2} s_x s_y \qquad (5.18) \\
& - \frac{t^4}{16U^3} \cos\Phi \sum_P \prod_{x \in P} s_x - \frac{5t^4}{16U^3} \cos\Phi \sum_P 1 + O(U^{-5})
\end{aligned}
$$

An analysis of the truncated effective potential to the order $O(U^{-5})$ yields the phase diagram of figure 7 for the ground states.
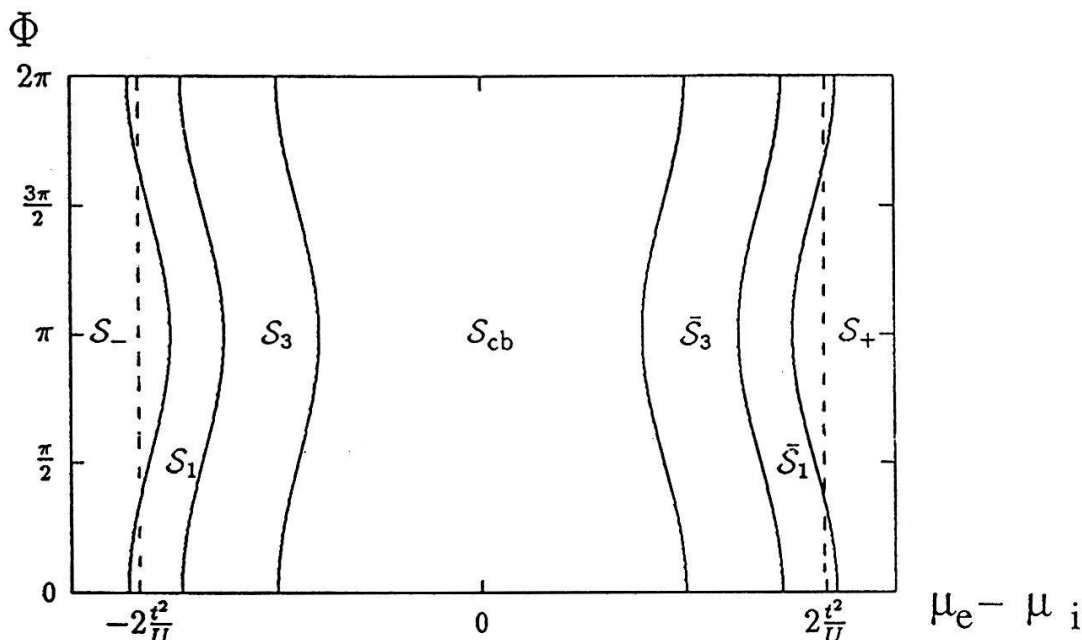

Figure 7: Phase diagram to order U^{-3} in the $(\mu_e - \mu_i, \Phi)$ plane, for the *square* lattice, and with hard-core *Bose* statistics. The dotted lines correspond to the phase diagram of the Ising model obtained to order U^{-1}.

This diagram is qualitatively similar to that of figure 4 for fermion systems and the same comments apply. For chemical potentials away from the boundaries in figure 7 one can rigorously establish that the configurations S_1, S_3, S_{cb} occur for U large. Therefore given the densities 1/5, 1/3, 1/2 and any flux Φ, we find the same configurations as in

the case of Fermi statistics. This suggests that the phase diagrams in the (ρ, Φ) plane, are identical for both kind of quantum statistics. On a triangular lattice this is definitely not the case (see below). Let us remark at this point that for $\mu_e = \mu_i = 0$ and $\Phi = 0$ reflection positivity implies that S_{cb} is the ground state for all U.

In [55] the same model was also considered on the triangular lattice. Now one has a particle hole symmetry, even though the lattice is not bipartite, and thus the phase diagram is symmetric with respect to $\mu_e - \mu_i = 0$ (see fig. 8 for the phase diagram to order U^{-2}). To order U^{-3} the boundary between diffrent domains open up and new phases appear (see [55]); in particular a phase with density $\rho_e = \rho_i = 1/2$ appears and for this density the ion configuration changes from T_8 to T_9 (see fig. 6) as the flux is varied. This feature was also present in the fermionic case. Moreover one remarks that for $(\rho = 1/2, \Phi = \pi/2)$, T_9 occurs for fermions whereas T_8 occurs for bosons (in fact this is true in a small region around the point $(1/2, \pi/2)$). Therefore for the triangular lattice the phase diagrams are different for each quantum statistic.
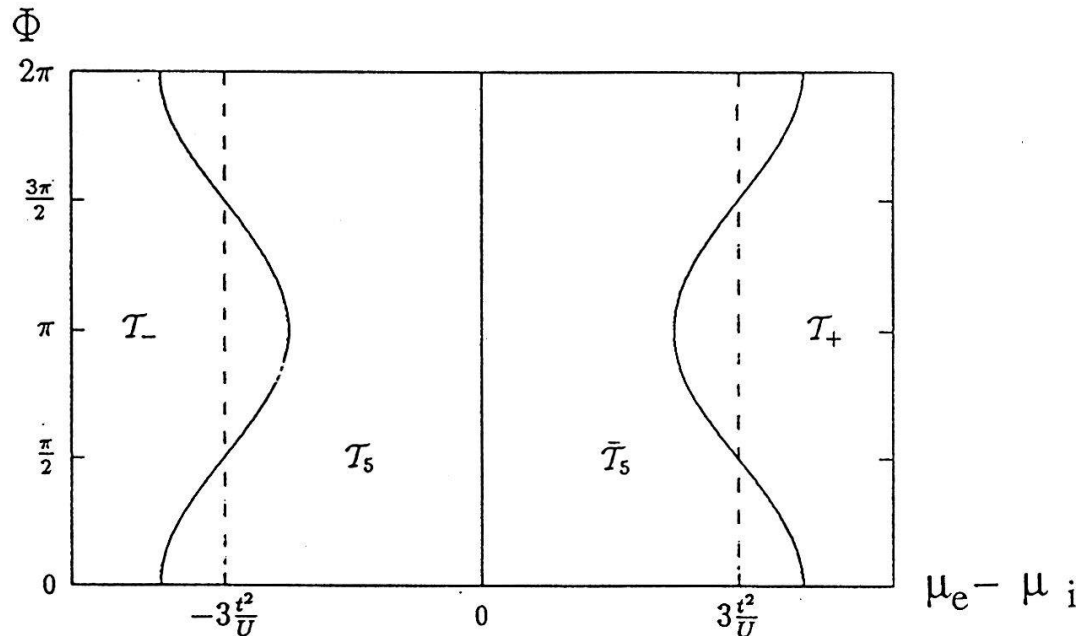

Figure 8: Phase diagram to order U^{-2} in the $(\mu_e - \mu_i, \Phi)$ plane, for the *triangular* lattice, and with hard-core *Bose* statistics. The dotted lines correspond to the phase diagram of the Ising model obtained to order U^{-1}.

To conclude this section let us mention that for any values (μ_e, μ_i), it follows from the functional integral representation that the optimal flux is zero for bosons. Note that this can also be checked directly on the U^{-1} expansions.

6. STATIC HOLSTEIN AND KONDO LATTICE MODELS

Some of the methods reviewed in sections 4 and 5 are not limited to the Falicov-Kimball model. Here we show how they can be applied to two other models, namely the static Holstein and the Kondo lattice models. Their common feature with the Falicov-Kimball model is that the itinerant electrons interact with a classical field by an on site potential. In the Falicov-Kimball model the classical field is a discrete spin $s_x = \pm 1$, whereas in the Holstein model it is a (scalar) continuous real unbounded variable. For the static Kondo lattice model we have a three component vector field on the unit sphere.

6.1 Static Holstein Model

This model is used to represent the interaction of electrons with an optical branch of phonons of a molecular crystal [78]. In the fully quantum Holstein model the phonons are treated like Einstein oscillators (representing internal vibration modes of some large molecules) attached to every site of the lattice. The static case corresponds to the classical limit for the oscillators. They are represented by a position variable s_x taking real unbounded values; usually the elastic energy of a configuration is proportional to $\sum_{x \in \Lambda} s_x^2$, but we consider the more general situation with anharmonic corrections $\sum_{x \in \Lambda} f(s_x^2)$ for some polynomial f. The coupling of the electrons to the phonons is linear. The hamiltonian that we consider is

$$H_\Lambda(\mathbf{s}) = - \sum_{x,y \in \Lambda} t_{xy} a_x^\dagger a_y + U \sum_{x \in \Lambda} s_x (a_x^\dagger a_x - \frac{1}{2}) + \sum_{x \in \Lambda} f(s_x^2) \qquad (6.1)$$

One can define the effective interaction F_Λ (in the grand canonical ensemble) by the formula (2.31) to which we add $\sum_{x \in \Lambda} f(s_x^2)$. The ground state energy E_Λ of a configuration $\mathbf{s}$ is found by taking the limit $\beta \to \infty$ of this expression. We note that the symmetry properties of the model are the same as that of the FK model, and $(\mu_e, \mu_i) = (0, 0)$ plays the same

role. Here μ_i fixes the position of the center of mass of the oscillators. In [65] the following results where proved for the symmetry point, on a lattice $\Lambda \subset \mathbf{Z}^d$ with $t_{<xy>} = 1$.

Theorem 6.1

Let $f(v)$ be a positive convex function for $v \geq 0$, with $f'(v) > 0$ for v large enough. Then (i) $E_\Lambda(\mathbf{s}, 0, 0)$ attains its global minimum for the chessboard configurations $s_x = \pm\epsilon_x \sigma_0(U)$ where $\sigma_0(U)^2$ is the solution of the equation in v

$$f'(v) = \frac{U^2}{4} \frac{1}{|\Lambda|} \sum_{k_\alpha, \alpha=1\ldots d} [e(k,v)]^{-1} \tag{6.2}$$

where

$$e(k,v) = \left[4 \left(\sum_{\alpha=1}^{d} cosk_\alpha \right)^2 + U^2 v \right]^{1/2} \tag{6.3}$$

and the sum is over the modes $k_\alpha = \pi n_\alpha/N$, $n_\alpha = -N, ..., N$, $(2N)^d = |\Lambda|$. (ii) These are the only two global minima.

This theorem makes rigorous the theory of the Peierls instability for this model. Here it is valid in all dimensions due to the fact that there is no dispersion for the phonons and we are at the symmetry point. Equation (6.2) is standard in the solid state literature and for the usual Holstein model where $f(v) = v$ the solutions behave (in the thermodynamic limit) as $\sigma_0(U) \sim U$ for large U and $\ln\sigma_0(U) \sim U^{-2}$ for small U (rigorous resuts on the Peierls instability also exist for other models, see [76,81]).

For other bipartite lattices and other fluxes there is a similar theorem with the appropriate dispersion relation replacing $\sum_{\alpha=1}^{d} cosk_\alpha$ in (6.2) (the lattice and t_{xy} have to be periodic). In this case the equation replacing (6.2) might not have a solution for all U. This happens for example on the cubic lattice with a flux equal to π per plaquette where the dispersion relation replacing $\sum_{\alpha=1}^{d} cosk_\alpha$ is $\sqrt{\sum_{\alpha=1}^{d}(cosk_\alpha)^2}$. One can show, in this case, that there is a solution for $U > U_c$ for some $U_c > 0$, while there is no solution for $U \leq U_c$ and the minimizing configuration is $s_x = 0$ for all $x \in \Lambda$. The same is true on the hexagonal lattice with a flux equal to zero per plaquette. We notice that this sensitivity of the minimizers on the lattice and the fluxes is absent in the FK model.

With the same setting as in theorem 6.1 we have also the following

Theorem 6.2

Let $f(v)$ be a positive convex polynomial $\sum_{j=1}^{N} a_j v^j$, with $a_N > 0$.

(i) If $a_1 = 0$, then for any β and U, $F_\Lambda(\mathbf{s}, \beta, 0, 0)$ attains its global minimum for $s_x = \pm \epsilon_x \sigma_1(U, \beta)$ where $\sigma_1(U, \beta)^2$ is the solution of the equation in v

$$f'(v) = \frac{U^2}{4} \frac{1}{|\Lambda|} \sum_{k_\alpha, \alpha=1...d} [e(k, v)]^{-1} \tanh[\frac{\beta}{2} e(k, v)] \tag{6.4}$$

Moreover these are the only two minima.

(ii) If $a_1 > 0$, then for a given U, equation (6.4) has a solution only for β large enough and the only global minima of $F_\Lambda(\mathbf{s}, \beta, 0, 0)$ are given by $s_x = \pm \epsilon_x \sigma_1(U, \beta)$

(iii) If all $a_j > 0$, $j = 1, ..., N$, then there exist a positive constant c such that for $\beta U^2 < c$, $F_\Lambda(\mathbf{s}, \beta, 0, 0)$ is a strictly convex function of s_x, which attains its minimum at $s_x = 0$, all $x \in \Lambda$.

This theorem gives a rather detailed picture of $F_\Lambda(\mathbf{s}, \beta, 0, 0)$ for the usual Holstein model which corresponds to (ii) and (iii). In that case the effective interaction has a "double well" structure for low temperatures with each well corresponding to the two chessboard configuration. At "high temperatures" ($\beta U^2 < c$) the double well disappears since the effective interaction becomes strictly convex. An application of the Brascamp-Lieb inequalities [79] shows that there is no long range order for $\beta U^2 < c$, in the following sense

$$\frac{1}{|\Lambda|} \sum_{x \in \Lambda} \sum_{y \in \Lambda} | < s_x s_y >_\Lambda (\beta)|^2 = O(1) \tag{6.5}$$

Finally the stability of the chessboard configurations with respect to thermal fluctuations was proved using a Peierls argument for continuous spins [65]. In other words there exist a fixed number δ of order $O(1)$ such that for U and β/U sufficiently large

$$\pm \sigma_0(U) - \delta \leq < \epsilon_x s_x >_\Lambda^\pm (\beta) \leq \sigma_0(U) + \delta \tag{6.6}$$

where $< - >_\Lambda^\pm$ is the thermal average with the appropriate boundary conditions, at the symmetry point.

6.2 Static Kondo Model

We consider the interaction of itinerant electrons with a periodic array of localised magnetic impurities. The electrons are spin one-half fermions and the spin of the magnetic impurities is treated classicaly, i.e. to each lattice site $x \in \Lambda$ we attach a normalised three component vector $\Phi_x = (\Phi_x^1, \Phi_x^2, \Phi_x^3)$, $|\Phi_x| = 1$. For a configuration of magnetic impurities $\Phi = \{\Phi_x\}$ the hamiltonian is

$$H_\Lambda[\Phi] = - \sum_{x,y \in \Lambda, \sigma = \uparrow, \downarrow} t_{xy} a_{x\sigma}^\dagger a_{y\sigma} + U \sum_{x \in \Lambda} S_x . \Phi_x \qquad (6.7)$$

with $S_x = (S_x^1, S_x^2, S_x^3)$, $S_x^i = \sum_{\gamma, \delta = \uparrow, \downarrow} a_{x\gamma}^\dagger \tau_{\gamma\delta}^i a_{x\delta}$, the electronic spin at site x, $\tau = (\tau^1, \tau^2, \tau^3)$ the Pauli matrices (5.3). The $|\Lambda| \times |\Lambda|$ matrix $\phi_x^i \delta_{xy}$ will be denoted simply by Φ^i. In fact $S_x . \Phi_x$ is the second quantisation of the matrix (it is a $2|\Lambda| \times 2|\Lambda|$ matrix acting on $\mathbf{C}^2 \otimes l^2(|\Lambda|)$)

$$\hat{\Phi} = \sum_{i=1}^3 \tau^i \otimes \Phi^i = \begin{pmatrix} \Phi^3 & \Phi^1 + i\Phi^2 \\ \Phi^1 - i\Phi^2 & -\Phi^3 \end{pmatrix} \qquad (6.8)$$

so that the one electron hamiltonian associated to (6.7) is

$$\hat{h}_\Lambda[\Phi] = -\hat{T} + U\hat{\Phi} \qquad (6.9)$$

where $\hat{T} = \mathbf{1}_2 \otimes T$, $\mathbf{1}_2$ the 2×2 identity matrix in spin space.

The grand canonical partition function is

$$Z_\Lambda(\beta, \mu_e, h) = \int_{|\Phi_x|=1} \prod_{x \in \Lambda} d\Phi_x \exp(-\beta F_\Lambda(\Phi, \beta, \mu_e, h)) \qquad (6.10)$$

where the effective interaction between the impurity spins is

$$\exp(-\beta F_\Lambda(\Phi, \beta, \mu_e, h)) = Tr \exp[-\beta(H_\Lambda - \mu_e N - h \sum_{x \in \Lambda} (\Phi_x + S_x^3))] \qquad (6.11)$$

In (6.10-6.11) the electronic chemical potential μ_e fixes the average density and h is an external magnetic field (along the third direction) coupled to the total spin (i.e. the electronic plus the impurity spin). We can perform the trace over the electrons in (6.11)

exactly and the result has the same form than (2.31) with $h_\Lambda(\mathbf{s})$ replaced by the hamiltonian (6.9). The ground state energy can then be defined as the limit of F_Λ as $\beta \to \infty$.

On a bipartite lattice the point $(\mu_e, h) = (0, 0)$ plays again a special role. At this point the effective interaction is invariant under $\Phi \to -\Phi$, so that $<\Phi_x>_\Lambda (\beta) = 0$ as in (2.38). Moreover using electron hole transformations on spin up and spin down electrons we can show that $<a^\dagger_{x\uparrow} a_{x\uparrow} + a^\dagger_{x\downarrow} a_{x\downarrow}>_\Lambda (\beta) = 1$. Thus at the symmetry point the system is half filled. The minimizers of $E_\Lambda(\mathbf{s}, 0, 0)$ and $F_\Lambda(\mathbf{s}, \beta, 0, 0)$ can easily be found to be the two Néel configurations. These are the configurations $\Phi_x = \epsilon_x \hat{n}$, $\hat{n}$ a given unit vector in $\mathbf{R}^3$. Let us illustrate this point more explicitly. On a bipartite lattice $\Lambda = A \cup B$ the unitary transformation $\epsilon_x \delta_{xy} \delta_{\gamma\delta}$ changes $\hat{T}$ to $-\hat{T}$ and leaves $\hat{\Phi}$ invariant so that by convexity (as in (4.1-4.2))

$$
\begin{aligned}
E_\Lambda(\Phi, 0, 0) &\geq -\frac{1}{2} tr\sqrt{\hat{T}^2 + U^2 \hat{\Phi}^2} \\
&= -\frac{1}{2} tr\sqrt{\hat{T}^2 + U^2}
\end{aligned}
\tag{6.12}
$$

In the last equality we use that $\hat{\Phi}^2 = \mathbf{1}$ as can be checked from (6.8). Now the lower bound in (6.12) is exactly the energy of a Néel state. Indeed $\hat{h}_\Lambda(\Phi)^2 = \hat{T}^2 + U^2 + (\hat{T}\hat{\Phi} + \hat{\Phi}\hat{T})$ with

$$
(\hat{T}\hat{\Phi} + \hat{\Phi}\hat{T}) = \begin{pmatrix} T\Phi^3 + \Phi^3 T & (T\Phi^1 + \Phi^1 T) + i(T\Phi^2 + \Phi^2 T) \\ (T\Phi^1 + \Phi^1 T) - i(T\Phi^2 + \Phi^2 T) & -T\Phi^3 - \Phi^3 T \end{pmatrix}
\tag{6.13}
$$

which is zero for a Néel state since

$$
(T\Phi^i + \Phi^i T)_{xy} = t_{xy} \hat{n}^i (\epsilon_x + \epsilon_y) = 0
\tag{6.14}
$$

Presumably the Néel state is stable with respect to thermal fluctuations in 3 dimensions, i.e. there is LRO, but the Kennedy-Lieb proof based on the Peierls argument, cannot be extended to this model because of the invariance of $F_\Lambda(\Phi, \beta, 0, 0)$ under global rotations of Φ. Of course one can perform U^{-1} expansions in the large U limit as for the FK model. To leading order one finds that the effective hamiltonian for the magnetic impurities is the classical Heisenberg antiferromagnet. For this model the occurence of LRO at low temperatures and in 3 dimensions has been proved by infrared bounds [80].

We also expect that the Néel state for the impurity spins, with an electronic density equal to one, persists close enough to the symmetry point in the (μ_e, h) plane, at least for

U large enough. If this is the case, the system is an insulator in the half filled band, at least for large U.

Finally we note that if we add a Hubbard type interaction between the electrons in (6.7), we can apply the reflection positivity techniques reviewed in section 5, to obtain results similar to those of the FK model. More precisely Theorem 5.1 is also valid with the Néel states replacing the chessboard states.

7. CONCLUSION

To conclude this review we want to mention a few open problems.

In one dimension it is known that for neutral systems with $\rho_e = \rho_i = p/q$, the ground state is given by the most homogeneous configuration (3.1) if $U > U_c(q)$ where $U_c(q)$ grows exponentially with q. The numerical analysis indicates that $U_c = t/\sqrt{3}$, but no proof has been found so far. Moreover it is expected that for $U > 2t$ these neutral states are the only (non trivial) pure states. For non neutral systems, and $U < 2t$, it is expected that for $\rho_e = p/q$, with p prime relative to q, and $\rho_i = p_i/q_i$ (p_i and q_i arbitrary) then the ground state is a mixture for $q_i \neq q$ and if a pure state exists for $q_i = q$, then it is given by (3.1), at least if $U < t\sqrt{3}$; this property has been established only in the limit $U \to 0$. In the grand canonical ensemble, it seems that the ground state can be classified according to the Farey tree rule for rational numbers [42,45]. For example it appears that the μ_e axis can be divided into intervals $I_{p,q}$ in which the most homogeneous configuration is the ground state for neutral systems with $\rho_e = \rho_i = p/q$, and such that the length $|I_{p,q}|$ is exponentialy decreasing with the level at which the rational p/q appears in the Farey tree. This rule can be checked for the first few rationals of the Farey tree using the U^{-1} expansion for large U, and numerical calculations for arbitrary U. A similar Farey structure also appears for $n-$ molecules ($\rho_i = n\rho_e$).

In two and three dimensions, going to higher orders in the U^{-1} expansion, a variety of new ground states appear and it is expected that for all densities there is a neutral (periodic) pure state, at least if U is sufficiently large. They seem to follow a composition rule similar to (3.1), with a Farey tree structure, and the appearance of $n-$ molecules for

small U [54].

The characterisation of the low temperature phase diagram has not yet been completed for the Falicov-Kimball model, except in the neigbourhood of the symmetry point. It is expected that this problem can be solved with the technique of [57] coupled to Pirogov-Sinai theory. For the static Holstein model at *small U*, the low temperature phase diagram has not been studied even at the symmetry point. The same is true for the static Kondo model of section 6, for all U. In this later case one has to deal with the continuous rotational symmetry, and the Peierls type arguments used for the other models do not work.

For the models of section 5 we have shown here that reflection positivity techniques can be applied (for special values of the flux) to find the ground state configurations at the symmetry point. Probably the only configuration that can be attained by this method is the chessboard because it is the only one which is invariant under all reflections. The occurence of long range order at low temperature can probably be studied at low temperature thanks to infrared bounds or chessboard estimates. However it is not clear how to prove these estimates because the interaction $s_x(n_{x\uparrow} + n_{x\downarrow})$ is purely on-site (for fermionic models with nearest neighbour interactions the infrared bound can easily be proven as pointed out in [70]). In any case it would be desirable to get results for *any* value of the flux, i.e. in cases where reflection positivity is not available.

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