Falicov-Kimball Models: A Partial Review of the Ground States Problem

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Abstract

In this review we present a biased review of the ground state properties of the Falicov-Kimball models in 1, 2 and ∞ dimensions, considering either fermions or hard core bosons. In particular we want to show the very rich structure that these models exhibit, and to point out the analogies and differences associated with the statistic of the quantum particles and the nature of the lattice (bipartite or not). The flux phase problem is also discussed.

Contents:

1 Introduction

1.1 Definition of the model

The Falicov-Kimball model is a *lattice model* of *quantum particules* interacting with *classical particles.*

The *lattice* $\Lambda = \{x\}$ is defined by a finite or infinite set of sites x in $\mathbb{R}^d$. Usually one considers d-dimensional cubic lattices $\mathbb{Z}^d$, and $\Lambda \subset \mathbb{Z}^d$. However it is interesting to consider more general lattices, e.g. the 2-d triangular lattice which, contrary to cubic lattices, is not bipartite. Indeed, particles on bipartite lattices have particle-hole symmetries, and one would like to know what properties remain valid for systems which do not have these symmetries. As we shall review, the rigourous results which have been obtained so far concern the cases where the coupling between quantum and classical particles is either very strong (in any dimension), or very weak (for d=1). For intermediate coupling, the only results concern reduced phase diagrams (sec. 1.4) and have been obtained using exact numerical methods. To investigate this intermediate coupling regime, it appears of interest to study first the model on the Bethe lattice in the limit where the coordination number becomes infinite; indeed in this limit one obtains a mean field model which should be simpler to study rigorously.

In the original model, the *quantum particles*, called "electrons" in the following, are spinless fermions described by creation and annihilation operators $a_x^\dagger, a_x$, satisfying the usual anticommutation relations

$$\{a_x, a_y\} = \{a_x^\dagger, a_y^\dagger\} = 0, \qquad \{a_x^\dagger, a_y\} = \delta_{x,y}. \tag{1}$$

It is well known that the Pauli principle is important to get a crystalline state, since such a state can not occur if fermions are replaced by bosons [4]. However hard-core bosons do indeed lead to crystaline structures [1] and they are interesting to study. Spinless hard-core bosons are described by operators $a_x^\dagger, a_x$ satisfying the following relations

$$\{a_x^\dagger, a_x\} = 1, \qquad \{a_x^\dagger, a_x^\dagger\} = \{a_x, a_x\} = 0 \tag{2}$$

but

$$[a_x^\#, a_y^\#] = 0 \quad \text{if} \quad x \neq y \qquad (a_x^\# = a_x^\dagger, a_x) \tag{3}$$

For the finite system Λ, the *kinetic energy* of the quantum particles is defined by the operator

$$K_\Lambda = -\sum_{x,y\in\Lambda} t_{xy}\, a_x^\dagger a_y \tag{4}$$

where $t_{xy} = t_{yx}^* = |t_{xy}|e^{i\theta_{xy}}$. Complex hopping constants t_{xy} are introduced to model particles in an external magnetic field: given a circuit $C = (x_1, x_2, \ldots, x_n, x_{n+1} = x_1)$, *i.e.* an ordered sequence of sites x_i in Λ such that $t_{x_i,x_{i+1}} \neq 0$ for all $i = 1, \ldots, n$, the magnetic flux through this circuit is defined by

$$\phi_C = \sum_{i=1}^{n} \theta_{x_i,x_{i+1}} \mod 2\pi. \tag{5}$$

In the original Falicov-Kimball model, only hopping between nearest-neighbour sites were considered, with

$$t_{xy} = \begin{cases} t \in \mathbb{R} & \text{if } |x-y| = 1 \\ 0 & \text{otherwise.} \end{cases} \tag{6}$$

Since then, several extensions of the model have been investigated, introducing quantum particles with "spin", described by operators $a^\dagger_{x\sigma}, a_{x\sigma}$, together with the kinetic energy

$$K_\Lambda = - \sum_{x,y \in \Lambda} \sum_{\sigma,\sigma'} t^{\sigma\sigma'}_{xy} \, a^\dagger_{x\sigma} a_{y\sigma'} . \tag{7}$$

For example, in the standard Hubbard model

$$K_\Lambda = - \sum_{x,y \in \Lambda} \sum_{\sigma=\uparrow,\downarrow} t_{xy} \, a^\dagger_{x\sigma} a_{y\sigma} . \tag{8}$$

For the asymmetric Hubbard model

$$K_\Lambda = - \sum_{x,y \in \Lambda} \sum_{\sigma=\uparrow,\downarrow} t^{\sigma}_{xy} \, a^\dagger_{x\sigma} a_{y\sigma} \tag{9}$$

with the Falicov-Kimball model given by

$$t^{\uparrow}_{xy} = t_{xy}, \quad t^{\downarrow}_{xy} = 0. \tag{10}$$

For the Montorsi-Rasetti model

$$K_\Lambda = - \sum_{x,y \in \Lambda} \sum_{\sigma,\sigma'=\uparrow,\downarrow} t_{xy} \, a^\dagger_{x\sigma} a_{y\sigma'} \tag{11}$$

and it has been shown that this model is equivalent to the Falicov-Kimball model.

The *classical particles*, called "ions" in the following, are assumed to have a hard-core. They are described by random variables $W_x \in \{0,1\}, x \in \Lambda$, where $W_x = 1$ means that the site x is occupied by an ion and $W_x = 0$ means that the site x is not occupied by an ion. In the spin-language, the random variable is s_x, where $s_x = 2W_x - 1 \in \{-1,+1\}$. The classical particles could be ions, impurities, spins, localised f-electrons, ..., depending on the physical system under investigation.

Again several extension have been considered. For example in the static Holstein model $s_x \in \mathbb{R}$ (and is associated with phonons), while in the static Kondo model $\boldsymbol{s}_x = (s^1_x, s^2_x, s^3_x) \in \mathbb{R}, |\boldsymbol{s}_x| = 1$, describes localized magnetic impurities.

The classical particles do not move and they do not have any kinetic energy. However in the definition of equilibrium states one will take annealed averages over all possible configurations of ions.

Except for the hard-core between ions, and the statistics for electrons, it is assumed that the only *interactions* are between electrons and ions when they occupy the same lattice site. It models for example the screened Coulomb interaction U which can be either positive (repulsion), ore negative (attraction). In other words, given the configurations $\boldsymbol{W} = \{W_x\}_{x\in\Lambda}$, or $\boldsymbol{s} = \{s_x\}_{x\in\Lambda}$, of the ions, the interaction is described by the operator

$$H_\Lambda^{\rm int}(\boldsymbol{W}) = 2U \sum_{x\in\Lambda} \left(W_x - \frac{1}{2}\right)\left(a_x^\dagger a_x - \frac{1}{2}\right) \tag{12}$$

or, equivalently,

$$H^{\rm int}(\boldsymbol{s}) = U \sum_{x\in\Lambda} s_x \left(a_x^\dagger a_x - \frac{1}{2}\right). \tag{13}$$

The factor $1/2$ is introduced for convenience to exhibit symmetry properties. In the canonical formalism it amounts simply to adding a constant; in the grand canonical formalism to a redefinition of the chemical potentials. In conclusion, given a configuration of the ions, the hamiltonian of the finite system Λ is given by

$$H_\Lambda(\boldsymbol{s}) = K_\Lambda + H_\Lambda^{\rm int}(\boldsymbol{s}) \tag{14}$$

to which is added in the grand canonical formalism the contribution

$$-\mu_e \sum_{x\in\Lambda} a_x^\dagger a_x - \mu_i \frac{1}{2} \sum_{x\in\Lambda} (s_x + 1), \tag{15}$$

with μ_e, μ_i the chemical potentials for electrons and ions.

Again several extensions can be considered. For example, for electrons with spins the following hamiltonian has been considered

$$H_\Lambda(\boldsymbol{s}) = K_\Lambda + U \sum_{x\in\Lambda} s_x \left(n_x - \frac{1}{2}\right) + U' \sum_{x\in\Lambda} \left(a_{x\uparrow}^\dagger a_{x\uparrow} - \frac{1}{2}\right)\left(a_{x\downarrow}^\dagger a_{x\downarrow} - \frac{1}{2}\right) \tag{16}$$

where $n_x = a_{x\uparrow}^\dagger a_{x\uparrow} + a_{x\downarrow}^\dagger a_{x\downarrow}$.

1.2 Interest of the Falicov-Kimball model

One of the most fundamental problem in condensed matter physics is to understand the phenomenon of phase transitions, in particular why all elements and many compounds crystallize in periodic structures. It is well known that one of the driving principles behind this ordering is associated with the structure of the ground states; however it is still not clear what physical mechanisms are necessary for phase transitions to occur, especially for quantum systems. Indeed, because of the quantum fluctuations, the ground state properties, as well as the low temperature behavior, are difficult to extract for quantum systems.

In 1969 Falicov and Kimball [5] introduced their model to study metal-insulator transitions in mixed valence compounds of rare earth and transition metal oxides as an effect of the interaction between localised f-electrons ("classical particles") and itinerant d-electrons (quantum particles). Later this same model was considered to study ordering in mixed valence systems, order-disorder transitions in binary alloys, and itinerant magnetism.

This model was reinvented in 1986 by Kennedy and Lieb [4] as a primitive model for matter to study crystallisation. In this interpretation ions are represented by classical particles and itinerant electrons by quantum particles. Depending on whether there is one, or several, electronic bands near the Fermi level, one is lead to consider neutral (equal density of ions and electrons), or non-neutral systems. For $\mu_e = \mu_i = 0$, which is the symmetry point of the system and corresponds to the neutral case with $\rho_e = \rho_i = \frac{1}{2}$, Kennedy and Lieb proved the existence of long range order (crystal) at low teperatures for any coupling U and any dimension $d \geq 2$, together with the absence of such order (fluid) at high temperatures. Their result was then extenden by J. L. Lebowitz and N. Macris in 1994 [6], for values of chemical potential in a neighborhood of the symmetry point.

1.3 Problems

The first step to study phase transitions is to obtain the zero temperature phase diagram, *i.e.* the ground states.

Problem 1: "Ground states" $(T = 0)$

Find the configuration of ions which minimize the energy.

Two approaches have been used to solve this problem.

In the *canonical formalism*, given (N_e, N_i), the number of electrons and ions, the problem is to find the configurations of ions $\boldsymbol{s} = \{s_x\}$ which minimize the energy, *i.e.*

$$E_{N_e}(\boldsymbol{s}) = \min_{\boldsymbol{s}':\ N_i(\boldsymbol{s}')=N_i} E_{N_e}(\boldsymbol{s}') \tag{17}$$

where $N_i(\boldsymbol{s}) = \frac{1}{2}\sum_{x\in\Lambda}(s_x + 1)$ and $E_{N_e}(\boldsymbol{s}')$ is the infimum of the spectrum of the hamiltonian $H_{\Lambda,N_e}(\boldsymbol{s}')$ restricted to the N_e electrons sector.

In the *grand canonical formalism*, given (μ_e, μ_i), the electron and ion chemical potentials, one starts from the partition function. Introducing an effective free energy $\mathcal{F}$ by means of a partial trace over the electrons degrees of freedom, *i.e.*

$$Z_\Lambda(\beta, \mu_e, \mu_i) = \sum_{\boldsymbol{s}} \mathrm{Tr}\{e^{-\beta[H_\Lambda(\boldsymbol{s}) - \mu_e N_e - \mu_i N_i(\boldsymbol{s})]}\} = \sum_{\boldsymbol{s}} e^{-\beta\mathcal{F}_\Lambda(\boldsymbol{s};\beta,\mu_e,\mu_i)} \tag{18}$$

one is lead to study a classical spin lattice system. Defining the effective hamiltonian for this classical spin system by

$$E_\Lambda(\boldsymbol{s}; \mu_e, \mu_i) = \lim_{\beta\to\infty} \mathcal{F}_\Lambda(\boldsymbol{s}; \beta, \mu_e, \mu_i) \tag{19}$$

the problem is to find those configurations of ions $\boldsymbol{s}$ which minimize $E_\Lambda(\boldsymbol{s}'; \mu_e, \mu_i)$, *i.e.* to find the zero temperature phase diagram of the effective hamiltonian.

Since the interaction is on-site, the quantum-mechanical problem for fermions can be solved by looking at the eigenvalues $e_j(\boldsymbol{s})$ of the hamiltonian $h_\Lambda(\boldsymbol{s})$ for one electron moving in the potential $U(s_x)$ defined by the configuration of ions. Therefore for *fermions systems*

$$E_\Lambda(\boldsymbol{s}_i;\mu_e,\mu_i) = \sum_{e_j(\boldsymbol{s})\leq\mu_e} [e_j(\boldsymbol{s})-\mu_e] - \frac{U}{2}\sum_x s_x - \mu_i N_i(\boldsymbol{s}) \tag{20}$$

$$= E_{N_e}(\boldsymbol{s}) - \mu_e N_e - \mu_i N_i(\boldsymbol{s}) \qquad \text{with } N_e = N_e(\mu_e). \tag{21}$$

On the other hand for systems of bosons with hard cores, we have a truly many-body problem of interacting particles; in this case one has to proceed via the effective free energy and the limit $\beta \to \infty$.

Problem 2: "Flux phases" $\quad (T=0)$
Let $\Phi = \{\phi_C\}$, where ϕ_C denotes the magnetic flux through the elementary circuit C.
The problems are the following:
i) Given (μ_e,μ_i,Φ), find the configurations of ions $\boldsymbol{s}$ which minimize $H_\Lambda(\boldsymbol{s};\Phi,\mu_e,\mu_i)$.
ii) Given (μ_e,μ_i), find the configurations $\boldsymbol{s}$ and the fluxes Φ which minimize $H_\Lambda(\boldsymbol{s};\Phi,\mu_e,\mu_i)$.

Problem 3: "Low themperature phase diagram"
The real problem in the study of phase transitions is to show that the zero temperature phase diagram is stable at low temperatures.

This question is discussed in the talks by R. Kotecky, D. Ueltschi, and N. Datta, and will not be considered in this review (see ref. [7]-[13]).

1.4 Methods

Several methods have been introduced to study the zero temperature phase diagram.

a) Expansion of $E_\Lambda(\boldsymbol{s};\mu_e,\mu_i)$ in powers of $|U|^{-1}$

This method has been introduced in both the canonical and the grand canonical formalism. It is valid in any dimension, but is restricted to

$$|U| > ct \quad \text{and} \quad \mu_e \in]-|U|+ct, |U|-ct[\tag{22}$$

where c is some constant depending on the lattice and $t = \max|t_{xy}|$. The conditions (22) imply in particular that this technique is restricted to

$$\text{"neutral" systems, } i.e.\ \ \rho_e = \rho_i, \qquad \text{if } U<0 \tag{23}$$

$$\text{"half-filled" systems, } i.e.\ \ \rho_e+\rho_i = 1, \quad \text{if } U>0 \tag{24}$$

where $\rho_e = \frac{N_e}{|\Lambda|}$ and $\rho_i = \frac{N_i}{|\Lambda|}$, are the (average) electrons and ions densities.

In the case of *fermions*, the expansion of $E_{N_e}(\boldsymbol{s})$ in powers of $|U|^{-1}$ is easily obtained using (20), together with the following property: with z the maximal coordination number of the lattice and $|U| > zt$, then, for any ions configuration $\boldsymbol{s}$, the spectrum of the 1-electron hamiltonian $h_\Lambda(\boldsymbol{s})$ has a gap containing the interval $]-|U|+zt, |U|-zt[$; for μ_e inside this gap the number of eigenvalues $e_j(\boldsymbol{s}) \le \mu_e$ is $N_i(\boldsymbol{s})$ if $U<0$ and $|\Lambda| - N_i(\boldsymbol{s})$ if $U>0$.

Therefore, for $N_e = N_i(\boldsymbol{s})$ if $U<0$, and for $N_e = |\Lambda| - N_i(\boldsymbol{s})$ if $U>0$, *i.e.* for μ_e in the above gap, we have

$$E_{N_e}(\boldsymbol{s}) = -\frac{U}{2}\sum_{x\in\Lambda} s_x + \frac{1}{2\pi i}\oint_C \mathrm{d}z \, \mathrm{Tr}\left\{\frac{z}{z-h_\Lambda(\boldsymbol{s})}\right\} \tag{25}$$

where C is a contour in the complex plane enclosing all negative eigenvalues.

Iterating the resolvent identiy for $[z-h_\Lambda(\boldsymbol{s})]^{-1}$ we obtain explicitely the desired expansion

$$E_{N_e}(\boldsymbol{s}) = \sum_{n\ge 1}\frac{1}{|U|^n}E_n(\boldsymbol{s}) \tag{26}$$

with

$$E_n(\boldsymbol{s}) = \sum_{x_1,\dots,x_{n+1}\in\Lambda} \frac{(-1)^m}{m}\frac{(n-1)!}{(m-1)!(n-m)!}\prod_{i=1}^{n+1} t_{x_i x_{i+1}} \tag{27}$$

where the sequence $(x_1,\dots,x_{n+1})$ must contain at least one emply site and one occupied site, and $m = m(\boldsymbol{s})$ is the number of sites $x_i, i = 1,\dots,n+1$, such that $s_{x_i} = -1$ if $U>0$, and $s_{x_i} = +1$ if $U<0$.

For *hardcore bosons*, the $|U|^{-1}$ expansion is obtained using the closed loop expansion of Messager-Miracle [12] for the effective free energy $\mathcal{F}(\beta;\boldsymbol{s},\mu_e,\mu_i)$. Taking the limit $\beta\to\infty$ yields the expansion for $E_\Lambda(\boldsymbol{s},\mu_e,\mu_i)$ which is convergent if the conditions (22) are satisfied, and implies the restriction Eq. (23), and (24).

In conclusion for both statistics we are able to write the effective hamiltonian as

$$E_\Lambda(\boldsymbol{s};\mu_e,\mu_i) = H^{(k)}(\boldsymbol{s};\mu_e,\mu_i) + R^{(k)}(\boldsymbol{s};\mu_e,\mu_i) \tag{28}$$

where

$$H^{(k)}(\boldsymbol{s};\mu_e,\mu_i) = H^{(0)}(\boldsymbol{s};\mu_e,\mu_i) + \sum_{n\ge 1}^{k}\frac{1}{|U|^n}E_n(\boldsymbol{s}). \tag{29}$$

At this point, the strategy is to study the ground states of the truncated hamiltonian $H^{(k)}$ and to control the rest $R^{(k)}$. With this technique one can prove that the phase diagram of the effective hamiltonian $E_\Lambda(\boldsymbol{s};\mu_e,\mu_i)$ is rigorously given by the phase diagram of the truncated hamiltonian, except for domains of width $|U|^{-(k+1)}$ (which can be explicitely estimated) centered on the boundaries of the phase diagram of $H^{(k)}$. At this order nothing can be said concerning (μ_e,μ_i) in these domains. Going to order $(k+1)$, the ground states of $H^{(k+1)}$ will give the ground states of $E_\Lambda(\boldsymbol{s};\mu_e,\mu_i)$ except for domains of width $|U|^{-(k+2)}$, and so on.

This method has been applied up to order $k=3$ to construct the phase diagrams for $d=1$ and 2, cubic and triangular lattices, both statistics, for systems with or without magnetic fields. However it is restricted by the conditions $\rho_e = \rho_i$ if $U<0$ and $\rho_e+\rho_i = 1$ if $U>0$.

b) Expansion of $E_\Lambda(\boldsymbol{s})$ in powers of $|U|$

This method has been used only in the canonical formalism. Contrary to the first method, it is valid for any rational densities (ρ_e, ρ_i) of electrons and ions, but so far it is restricted to 1 dimension only.

Assuming $t_{xy} = t \neq 0$ only if $|x-y| = 1$, then, using Rayleigh-Schrödinger perturbation theory, one obtains for the ground state energy density (for $U < 0$)

$$e(\boldsymbol{s};\rho_e) = 2\rho_e - \frac{2t}{\pi}\sin\pi\rho_e - U\rho_e\rho_i + \frac{1}{4\pi t}\frac{|W_q|^2}{\sin\pi\rho_e}U^2\ln|U| + O(U^2) \tag{30}$$

where $\rho_e = p/q$ (p prime with respect to q) and

$$W_q(\boldsymbol{s};\rho_e) = \frac{1}{q}\sum_{x=0}^{q-1} e^{-i2\pi\rho_e x} s_x. \tag{31}$$

Given $\rho_e = p/q$, the problem is then to find the configurations $\boldsymbol{s}$ which minimize $e(\boldsymbol{s};\rho_e)$.

c) Reduced phase diagrams

This method is valid for arbitrary coupling constant U and arbitrary densities (ρ_e, ρ_i), resp. (μ_e, μ_i), but gives only qualitative results. The idea is to select some restricted class of ions configurations, e.g. all periodic configurations with period ≤ 16 together with mixtures of two such periodic configurations, and to search, by means of exact numerical computation, for the configurations in this class which minimize the energy. This yields the so called reduced phase diagram. It has been applied in 1 and 2 dimensions.

From these numerical calculations, one observes that this approach yields results consistent with those rigorously established in the limit of large or small U. Moreover the reduced phase diagram appears rather stable, *i.e.* increasing the class of configurations considered, the boundaries of the previous reduced phase diagram become domains of smaller and smaller width, where new ground states configurations appear, while the main part of the diagram is not modified. The situation is similar to the case discussed above, passing from the truncated hamiltonian $H^{(k)}$ to $H^{(k+1)}$.

d) Finite systems

In 1 and 2 dimensions explicit numerical computations of the energies have been developped to find the exact ground state configurations of some finite systems. In fact, it is this early approach which led to the conjecture of "molecule formation" and to the idea, later proved, that for small $|U|$ and small densities (e.g. $\rho_e = \rho_i < \frac{1}{4}$) the ground state is not periodic.

2 Results for 1-dimensional systems

In 1 dimension, using the closed loop expansion for the effective free energy, one first concludes that hard core bosons are identical to fermions [2].

In the following we consider only the attractive case $U < 0$. From particle-hole symmetry one then obtains similar conclusion for $U > 0$.

Using the canonical formalism, the following results were obtained.

Theorem 1 (Strong coupling [14])

a. Let $\rho_e = \rho_i = p/q$, with p prime with respect to q, then for $|U| > U_{cr}(q)$ the ground state is the most homogeneous periodic configuration *with period q. The position of the ions on the sites $(0, 1, \ldots, q-1)$ is given by $W_x = 1$ for $x = k_j$ where k_j is solution of the equation*

$$pk_j = j \mod q \qquad j = 0, 1, \ldots, p-1. \tag{32}$$

b. Let $\rho_i = b\rho_e, b \neq 1$, then for $|U| > U_{seg}(b)$ the ground state is the segregated configuration *where all ions clump together.*

Theorem 2 (Weak coupling [15])

Given $\rho_e = p/q$ with p prime with respect to q, and $|U| \ll q$, then

a. for $\rho_i \in]\frac{p'}{q}, \frac{p'+1}{q}[$, the ground state is a mixture *of two periodic configurations $\boldsymbol{s}'$ and $\boldsymbol{s}''$, with $\rho_i' = \frac{p'}{q}$, $\rho_i'' = \frac{p'+1}{q}$ ($\rho_e' = \rho_e'' = p/q$), where the position of ions is given by eq. (32), with $j = 0, 1, \ldots, p'-1$ (resp. $j = 0, 1, \ldots, p'$).*

b. for $\rho_i = p_i/q$, p_i not necessarily prime with respect to q,

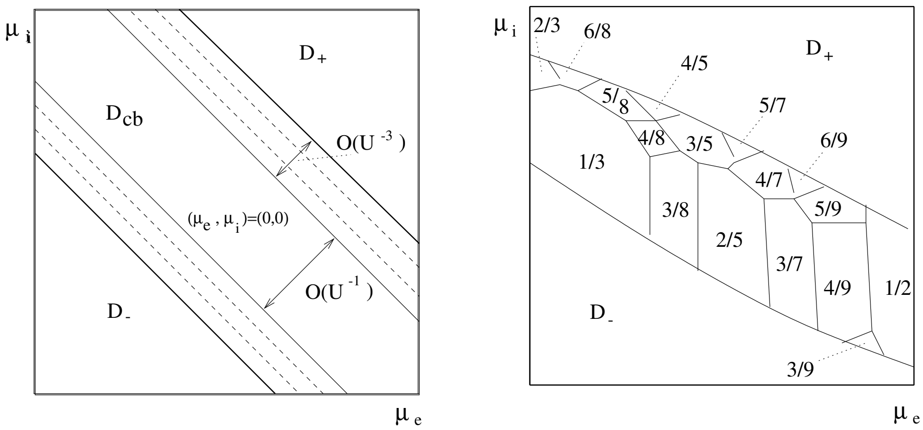
1. *if $\rho_i \in]0.37, 0.63[$, the ground state is the* periodic *configuration of period q, given by eq. (32).*
2. *if $\rho_i < 0.37$, or $\rho_i > 0.63$, the ground state is a* mixture *consisting of a periodic configuration, with period q and ion density $\rho_i' = p_i'/q$, solution of eq. (32), together with empty ($\rho_i'' = 0$) or full ($\rho_i'' = 1$) configuration (and $\rho_e' = \rho_e'' = p/q$),* except *for a countable set of densities (ρ_e, ρ_i), with $\rho_i \in [\frac{1}{4}, 0.37] \cup [0.63, \frac{3}{4}]$, where the ground state is the periodic ground state, with period q, given by eq. (32). This countable set is given by the solutions of an equation, and we have for example*

$$\rho_i = \rho_e = \frac{1}{4}, \frac{1}{3}, \frac{7}{20}, \frac{6}{17}, \frac{14}{39}$$
$$\rho_i = 2\rho_e = \frac{1}{3}, \frac{6}{17}, \frac{10}{18}, \frac{14}{39}, \ldots$$

This property shows that the periodicity of the pure phase is fixed by the electron density: it is the smallest period necessary to open a gap at the Fermi level. Let us also remark that the critical ion densities given above (*i.e.* $\rho_i = 0.37$ and 0.63) are approximate values. The exact values are ρ_c and $(1 - \rho_c)$, with ρ_c solution of $2\pi\rho_c = \tan \pi\rho_c$.

The results of theorem 2 show that there is a close analogy with the Peierls instability; however this analogy is valid only for $\rho_i \in [\rho_c, 1-\rho_c]$ and can be seen as follows: For $U = 0$ ($\rho_e = p/q, \rho_i = p_i/q$ fixed) any ions configuration is a ground state and the probability to find an ion at a given site is uniform, equals to ρ_i. This is the "undistorted state", which is metallic (no gap). For $U \neq 0$, sufficiently small, a particular configuration is selected which has period q. It corresponds to the "distorted state", which has a gap at the Fermi level and is insulating. For $\rho_i \notin [\rho_c, 1-\rho_c]$ the ground state is a mixture of a metallic and insulating phase (except for exceptional densities) and such a situation does not occur in the standard theory of Peierls and Fröhlich.

To extend these investigations to arbitrary values of the coupling constant U, and to avoid difficulties associated with mixtures, it is more convenient to work in the grand canonical formalism. Reduced phase diagrams were obtained in [16] for several values of U, by means of exact numerical calculations. Some examples are illustrated on figure 1.



(a) Strong coupling

(b) Weak coupling

Figure 1

Figure 1a) shows part of the chemical potential plane for strong coupling, *i.e.* $U < 2t$. D_-, D_+, D_{cb} represent domains where the ground state is the empty ($\rho_i = 0$) , the full ($\rho_i = 1$), and the chessboard configuration. The parallel stripes corresponds to domains with $\rho_e = \rho_i =$ const.

Figure 1b) shows part of the chemical potential plane for weak coupling, *i.e.* $U \in [-2t, 0]$. The "vertical" stripes with same denominator q correspond to periodic ground states with fixed electron density $\rho_e = p/q$ and different ion densities $\rho_i = p_i/q$.

Combining all the results obtained so far, either rigorously or by reduced phase diagrams analysis, one is led to the following conclusion

Conjecture *Given the electron density $\rho_e = p/q$, p prime with respect to q, and the ion density $\rho_i = p_i/q$, p_i not necessarily prime with respect to q, if the ground state is periodic then it has period q and the position of the ions is given by the solutions of the equation*

$$pk_j = j \mod q, \qquad j = 0, 1, \ldots p_i - 1. \tag{33}$$

In all other cases, the ground state is either

1. *a mixture of two periodic configurations with* $\rho_i = p_i/q$ *and* $\rho_i = (p_i + 1)/q$ *given by the solutions of eq.* (33)

2. *a mixture of one periodic configuration solution of eq.* (33), *together with either the empty* ($\rho_i = 0$) *or the full* ($\rho_i = 1$) *configuration.*

3. *the segregated configuration.*

Let us remark that eq. (33) is reminiscent of the circle map theorem, and appears in many situations.

3 Results for two dimensional systems

The ground state properties of the Falicov-Kimball model on the square lattice, in the limit of strong coupling, are discussed in the talk by T. Kennedy.

Reduced phase diagram analysis for the square lattice and arbitrary values of the coupling U has been conducted by Watson and Lemanski [17], [18]. Their results show that the properties discussed in sec. 2 are not specific to one dimensional systems, but also appears (together with new properties) in two dimensions.

In this section we want to exhibit the difference between fermions and hard-core bosons, between square and triangular lattices, and to discuss the flux phase problem.

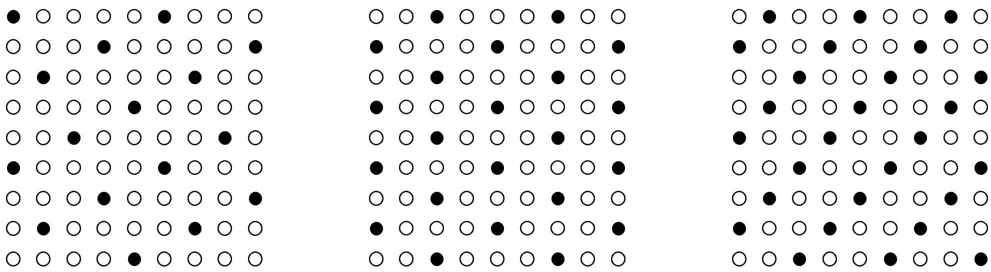
This analysis has been conducted, within the grand canonical formalism, in the limit of strong coupling, using the $|U|^{-1}$ expansion discussed in sec. 1.4. It is thus restricted to neutral (if $U < 0$) or half-filled (if $U > 0$) systems (ref. [2], [19]).

The phase diagrams for fermions and hard-core bosons in the presence of an homogeneous magnetic field, defined by its flux Φ through elementary cells (in particular it could be zero), are represented on figures 2a and 2b for the square lattice, and on figures 4a and 4b for the triangular lattice. These phase diagrams are those of the truncated hamiltonians; the exact phase diagrams are identical except for small domains around the boundary curves which have been explicitely evaluated [2].

(a) Phase diagram to order 3 for fermions on the square lattice

(b) Phase diagram to order 3 for hard-core bosons on the square lattice

Figure 2



$\mathcal{S}_1,\ \rho = \frac{1}{5}$ $\mathcal{S}_2,\ \rho = \frac{1}{4}$ $\mathcal{S}_3,\ \rho = \frac{1}{3}$

Figure 3: Configurations S_1, S_2, S_3 which appears in fig. 2 (a) and (b). $\bar{S}_1, \bar{S}_2, \bar{S}_3$ are obtained by particle-hole transformation. $S_-, S_+, S_{\rm cb}$ are respectively the empty ($\rho = 0$), the full ($\rho = 1$), and the chessboard ($\rho = \frac{1}{2}$) configurations.

(a) Phase diagram to order 2 for fermions on the triangular lattice.

(b) Phase diagram to order 2 for hard-core bosons on the triangular lattice.

Figure 4

In fig. 4 (a) and (b), τ_- and τ_+ are the empty ($\rho = 0$) and full ($\rho = 1$) configurations; τ_5 and $\bar{\tau}_5$ are the periodic configurations with densities $\frac{1}{3}$ and $\frac{2}{3}$.

The analysis of the triangular lattice has been extended to order 3. At this order the phase diagramms exhibit periodic configurations with densities $\rho = (0, \frac{1}{7}, \frac{1}{5}, \frac{1}{4}, \frac{1}{4}, \frac{1}{3}, \frac{2}{5}, \frac{4}{9}, \frac{1}{2}, \frac{1}{2})$ as well as $(1 - \rho)$. We note that there exist two different structures with densities $\frac{1}{4}$, and with density $\frac{1}{2}$. The interested reader should consult the original article [2].

It remains to discuss the flux phase problem. In particular one would like to know in what cases, if any, the magnetic flux will decrease the energy of the system, and what is the optimal magnetic flux to obtain the state of minimum energy, *i.e.* the ground state.

For hard-core bosons it is easy to see that the optimal magnetic flux is always zero (diamagnetic inequality) [2].

For fermions the situation is more subtle; it depends on the lattice and the densities. On the square lattice, one finds that for density $\frac{1}{2}$ the optimal flux is $\phi = \pi$ through each plaquette, and the ion configuration is the chessboard structure; for densities $\frac{1}{3}$ and $\frac{2}{3}$ the optimal flux is no longer uniform but periodic with period 3, and $\phi = 0$ or π (the ion configurations are the structures $S_3, \bar{S}_3$ of figure 5); similarly for densities $\frac{1}{5}$ and $\frac{4}{5}$, at order 3 the optimal flux is non uniform, but periodic with $\phi = 0$ or arbitrary (and the configurations are $S_1, \bar{S}_1$); for densities 0 and 1, the fluxes are arbitrary. We note that at this order the configurations with densities $\frac{1}{4}$ and $\frac{3}{4}$ do not appear (but they might appear at the next order however). We also should remark that on the square lattice the optimal flux is maximum (*i.e.* $\phi = \pi$ everywhere) for density $\rho = \frac{1}{2}$, which is the maximum possible density, because of the particle-hole symmetry.

The situation is very different for the triangular lattice. One finds that the optimal flux is maximum ($\phi = \pi$ everywhere) for densities $\rho = \frac{1}{4}, \frac{1}{3}, \frac{2}{3}, \frac{3}{4}$; however for density $\rho = \frac{2}{5}, \frac{1}{2}, \frac{3}{5}$, the optimal flux is not uniform, but periodic, with $\phi = 0$ or π. (Let us recall that on the triangular lattice the particle-hole transformation is not a symmetry). Similarly for densities $\rho = \frac{1}{7}$ and $\frac{5}{7}$, the optimal flux is not uniform, but periodic, with $\phi = 0$ or arbitrary (this arbitrariness may be lifted at the next order); finally for densities 0 and 1, the fluxes are arbitrary.

The results for the flux phase problem are illustrated on figure 5.

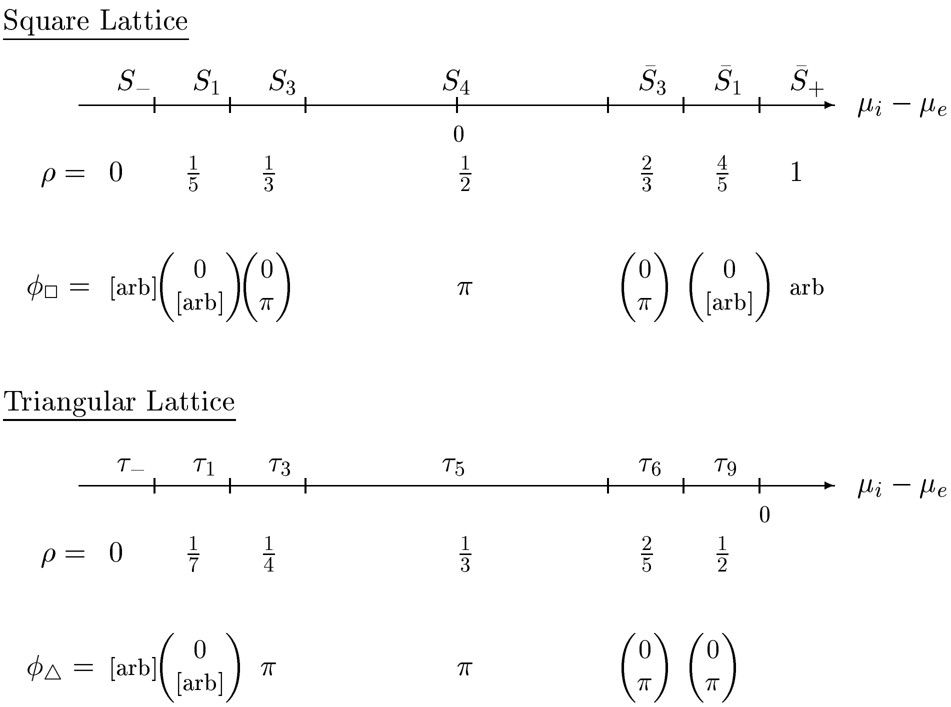


Figure 5: Optimal magnetic fluxes, [arb] means arbitrary at order 3, $\rho_i = \rho_e = \rho$.

We conclude this discussion with the following theorem [2].

Theorem 3 *For fermions systems*

1. *for the configurations* $s_+ = \{s_x = +1\}$ *and* $s_- = \{s_x = -1\}$*, the effective hamiltonian is independant of the magnetic fluxes.*

2. *for any configuration* $\boldsymbol{s} \neq s_+$ *and* s_-*, there exists* $U_0(\boldsymbol{s})$ *such that for* $U \geq U_0(\boldsymbol{s})$*, the optimal fluxes (*i.e. *those wich minimize the energy) are*

   (a) for the square lattice

$$\phi_{\square}^{min}(\boldsymbol{s}) = \begin{cases} \pi & \text{if 2 sites of } \square \text{ are occupied} \\ 0 & \text{otherwise} \end{cases} \tag{34}$$

   (b) for the triangular lattice

$$\phi_{\triangle}^{min} = \begin{cases} \pi & \text{if 0 or 1 site of } \triangle \text{ are occupied} \\ 0 & \text{otherwise} \end{cases} \tag{35}$$

4 Preliminary results for ∞-dimension Bethe lattice system

In this section, the system is defined on the Bethe lattice with coordination number z (fig. 6) and by the hamiltonian

$$H(\boldsymbol{W}) = -\sum_{x,y} t_{xy}\, a_x^\dagger a_y + U \sum_x W_x a_x^\dagger a_x \tag{36}$$

with $W_x \in \{0, 1\}$ and

$$t_{xy} = t_{yx} = \begin{cases} \frac{t}{\sqrt{z}} & \text{if } |x-y| = 1 \\ 0 & \text{otherwise} \end{cases} \tag{37}$$

We shall then consider the limit $z \to \infty$. The Falicov-Kimball model on this infinite dimensional Bethe lattice has attracted a considerable interest since 1989 and the reader should consult the references [22], [23] for more informations.

The density of electrons on the site x is expressed as

$$\left\langle a_x^\dagger a_x \right\rangle (\beta, \mu_e, \mu_i) = \frac{1}{\beta} \sum_n G_{nn}(\omega_n) \tag{38}$$

with $\omega_n = \frac{\pi}{\beta}(2n+1)$ the Matsubara frequencies.

The strategy proceeds as follows. Using

1. Grassmann variables

2. the fact that H is quadratic in $a_x^\dagger, a_x$

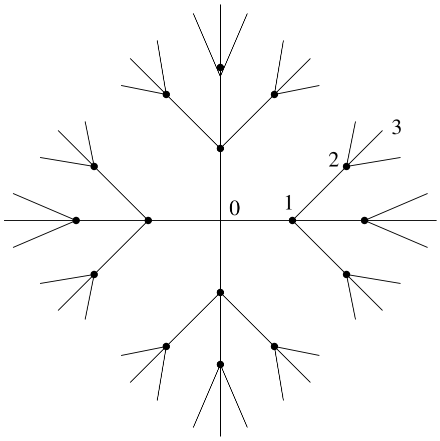


Figure 6: Bethe lattice. The shells $l = 0, 1, 2, 3$ are represented.

3. the fact that there are no closed loop on Bethe lattice and introducing the complex variable

$$\xi_n = i\omega_n - \mu_e \tag{39}$$

we obtain the explicit expression

$$G_{xx}(\omega_n) = \frac{\langle W_x \rangle - 1}{\xi_n + I_x(\omega_n)} - \frac{\langle W_x \rangle}{\xi_n + U + I_x(\omega_n)} \tag{40}$$

where

$$I_x(\omega_n) = \frac{1}{2} \sum_{y:|x-y|=1} t^2 G_{yy}^{\Lambda \setminus x}(\omega_n) \tag{41}$$

($\Lambda \setminus x$ is the Bethe lattice with the site x deleted) and

$$\langle W_x \rangle = \left[1 + e^{-\beta(\mu_i - Y_x(\beta,\mu_e))}\right]^{-1} \tag{42}$$

$$Y_x(\beta, \mu_e) = \frac{1}{\beta} \sum_n \{\ln[\xi_n + I_x(\omega_n)] - \ln[\xi_n + U + I_x(\omega_n)]\} \tag{43}$$

4. At this point one takes the thermodynamic limit in a symmetrical manner, by increasing to infinity the number of shells. In this limit

$$G_{xx}(\omega_n) = G_l(\omega_n), \qquad \langle W_x \rangle = \alpha_l \tag{44}$$

where $l = 0, 1, 2, \ldots$ denotes the shells ($l = 0$ is the center point, $l = 1$ are the z nearest neighbours, and so on).

5. Taking the limit of infinite dimension, $z \to \infty$, we have from (41) and (40)

$$I_x(\omega_n) = I_l(\omega_n) = t^2 G_{l+1}(\omega_n) \tag{45}$$

$$G_l(\omega_n) = \frac{\alpha_l - 1}{\xi_n + t^2 G_{l+1}(\omega_n)} - \frac{\alpha_l}{\xi_n + U + t^2 G_{l+1}(\omega_n)} \tag{46}$$

$$\alpha_l = \left[1 + e^{-\beta(\mu_i - Y_x(\beta,\mu_e))}\right]^{-1} \tag{47}$$

6. We can then take the zero temperature limit $\beta \to \infty$, to obtain

$$Y_l(\mu_e) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega \, \{\ln[\xi + t^2 G_{l+1}(\omega)] - \ln[\xi + U + t^2 G_{l+1}(\omega)]\} \tag{48}$$

7. We thus conclude from (47) that in the limit $\beta \to \infty$

$$\text{either } \alpha_l = 0 \quad \text{and this happens iff } Y_l(\mu_e) > \mu_i \tag{49}$$

$$\text{or } \alpha_l = 1 \quad \text{and this happens iff } Y_l(\mu_e) < \mu_i \tag{50}$$

8. The problem is reduced to the following ones:
Given $\boldsymbol{\alpha} = [\alpha_0, \alpha_1, \dots, \alpha_{p-1}], \alpha_\rho \in \{0, 1\}$,

   (a) show that eq. (46) has a unique solution, $G_l(\omega_n), l = 0, 1, \dots, n-1$

   (b) from $G_l(\omega_n)$ and eq. (48) determines $Y_l(\mu_e)$

   (c) Using eq. (49) find those (μ_e, μ_i) for which the "periodic" configuration $\boldsymbol{\alpha}$ (periodic with respect to successive shells) is the ground state.

With this procedure, the following result was obtained ([20], [21]).

Theorem 4 *For $\mu_e \in]2t, U-2t[$, then*

- *for $\mu_i - \mu_e < -t^2/U$, the ground state is the empty configuration ($W_x = 0$).*
- *for $\mu_i - \mu_e > t^2/U$, the ground state is the full configuration ($W_x = 1$).*
- *for $\mu_i - \mu_e \in [-A, A]$, with*

$$A = \frac{t^2}{U} - 4\frac{t^4}{U^3} + 27\frac{t^6}{U^5} + O(\frac{t^8}{U^7}) \tag{51}$$

  the ground states are the period 2 configurations $\boldsymbol{\alpha} = [0, 1]$, and $\boldsymbol{\alpha} = [1, 0]$.

- *for $\mu_i - \mu_e \in [-B, -A]$, and for $\mu_i - \mu_e \in [A, B]$ with*

$$B = \frac{t^2}{U} - 6\frac{t^6}{U^5} + O(\frac{t^8}{U^7}) \tag{52}$$

  the ground states are the period 3 configurations given respectively by $\boldsymbol{\alpha} = [0, 0, 1]$, $[0, 1, 0]$, $[1, 0, 0]$ and by $\boldsymbol{\alpha} = [0, 1, 1], [1, 0, 1], [1, 1, 0]$.

5 Conclusion

Although extremly simple in its formulation, the Falicov-Kimball models exhibit a very rich structure in all dimension. In particular, on can prove

- Periodic ground states
- Molecules formation
- Segregation
- Coexistence of phases
- Metal-insulator transition
- Peierls instability
- Devil staircase (maybe complete)
- Farey tree properties
- Flux phases

Among the open problems, on can mention the following

- Prove the conjecture for 1-dimensional systems
- Find the exact equation for the segregated configuration (1-dim)
- Find the conditions for the ground state to be periodic (in any dimension)
- Prove the devil staircase structure
- Find the low temperature properties
- Find the thermodynamic properties of the general class of system consisting of quantum particles interacting with classical fields.

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A large number of references concerning the Falicov-Kimball model in 1 and 2 dimensions can be found in [1] and [2] below and will not be reproduced here, unless quoted in the text.

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